Serial Number 09/937,122

Access DB# 91706

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Keith Levy Examiner #: 72604 Date: 4/14/03

Art Unit: 2625 Phone Number 30 605 1153 Serial Number: ~~09/937,122~~

Mail Box and Bldg/Room Location: 3D01-4A16 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: See previous copy

Inventors (please provide full names):

Earliest Priority Filing Date:

For Sequence Searches Only *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Rejected

****

STAFF USE ONLY

Searcher: Alexandra Waclawiw

Searcher Phone #: CA02 Tel: 308-4491

Searcher Location:

Date Searcher Picked Up: 4-17-03

Date Completed: 4-17-03

Searcher Prep & Review Time:

Clerical Prep Time:

Online Time:

Type of Search		Vendors and cost where applicable	
NA Sequence (#)		STN	496.00
AA Sequence (#)		Dialog	
Structure (#)	1	Questel/Orbit	
Bibliographic		Dr.Link	
Litigation		Lexis/Nexis	
Fulltext		Sequence Systems	
Patent Family		WWW/Internet	
Other		Other (specify)	

RECEIVED APR 15 2003 TECH CENTER 2600

PTO-1590 (8-01)

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=> d his

     (FILE 'REGISTRY' ENTERED AT 08:18:37 ON 17 APR 2003)
                DEL HIS Y
                E 1,3-BUTADIENE/CN
L1            2 S E3-4
                E METHYL PENTENOATE/CN
L2            1 S E3
                E PENTENOIC ACID, METHYL ESTER/CN
L3            3 S E3-5
L4            3 S L2 OR L3
                E METHYL ADIPATE/CN
L5            2 S E3
                ACT CATALYST/A
               ---------
L6              STR
L7              SCR 2017 AND 1839
L8         3282 SEA FILE=REGISTRY SSS FUL L6 AND L7
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     FILE 'HCAPLUS' ENTERED AT 08:28:01 ON 17 APR 2003

     FILE 'REGISTRY' ENTERED AT 08:28:10 ON 17 APR 2003
                E CARBON MONOXIDE/CN
L9            1 S E3

     FILE 'HCAPLUS' ENTERED AT 08:28:18 ON 17 APR 2003
L10      119149 S L1 OR BUTADIENE
L11         703 S DIENE# (L) CARBONYL?
L12        1491 S L8
L13          22 S L10 AND L12
L14           4 S L11 AND L12
L15          22 S L14 OR L13
L16        1374 S L4 OR L5
L17      119687 S L10 OR L11
L18          64 S L17 AND L16
L19          35 S L18 AND (CATALY? OR CAT/RL)
L20          20 S L19 AND CARBONYL?
L21      260284 S L9 OR CARBON DIOXIDE#
L22          21 S L21 AND L19
L23          13 S L22 AND L20
L24          10 S L23 NOT L15
L25           1 S L24 AND (P OR PHOSPHOR? OR PHOSPHOR?/AB)
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=> fil reg
FILE 'REGISTRY' ENTERED AT 08:32:15 ON 17 APR 2003
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   16 APR 2003  HIGHEST RN 503266-82-8
DICTIONARY FILE UPDATES:  16 APR 2003  HIGHEST RN 503266-82-8

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d que l1;d l1
L1             2 SEA FILE=REGISTRY ABB=ON  PLU=ON  ("1,3-BUTADIENE"/CN OR
                 "1,3-BUTADIENE CATION RADICAL"/CN)

L1   ANSWER 1 OF 2  REGISTRY  COPYRIGHT 2003 ACS
RN   34488-62-5  REGISTRY
CN   1,3-Butadiene, radical ion(1+) (9CI)  (CA INDEX NAME)
OTHER NAMES:
CN   1,3-Butadiene cation radical
CN   1,3-Butadiene radical cation
CN   Butadiene cation radical
CN   Butadiene radical cation
CN   Butadiene radical ion(1+)
MF   C4 H6
CI   COM, RIS
LC   STN Files:   BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER
         (*File contains numerically searchable property data)
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$H_2C{=}CH{-}CH{=}CH_2$

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              87 REFERENCES IN FILE CA (1962 TO DATE)
               2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
              87 REFERENCES IN FILE CAPLUS (1962 TO DATE)


=> d que l4;d l4 1-3
L2             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  "METHYL PENTENOATE"/CN
L3             3 SEA FILE=REGISTRY ABB=ON  PLU=ON  ("PENTENOIC ACID, METHYL
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also this was searched RW = 106-99-0 forgot to print, see printout in references

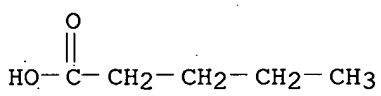
ESTER"/CN OR "PENTENOIC ACID, METHYL ESTER, ISOMER"/CN OR "PENTENOIC ACID, METHYL-, (Z)-"/CN)

L4 3 SEA FILE=REGISTRY ABB=ON PLU=ON L2 OR L3

L4 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2003 ACS
RN 83582-32-5 REGISTRY
CN **Pentenoic acid, methyl-, (Z)- (9CI)** (CA INDEX NAME)
MF C6 H10 O2
CI IDS
LC STN Files: CA, CAPLUS

CM 1

CRN 27936-41-0
CMF C6 H12 O2
CCI IDS



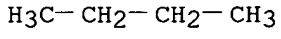
D1—Me

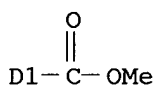
1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L4 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2003 ACS
RN 68393-76-0 REGISTRY
CN **Pentenoic acid, methyl ester, isomer (9CI)** (CA INDEX NAME)
MF C6 H10 O2
CI IDS
LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 68393-75-9
CMF C6 H12 O2
CCI IDS



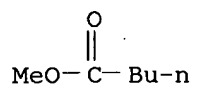


1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L4 ANSWER 3 OF 3 REGISTRY . COPYRIGHT 2003 ACS
RN 30644-57-6 REGISTRY
CN **Pentenoic acid, methyl ester (7CI, 9CI)** (CA INDEX NAME)
OTHER NAMES:
CN **Methyl pentenoate**
MF C6 H10 O2
CI IDS
LC STN Files: ANABSTR, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPATFULL

CM 1

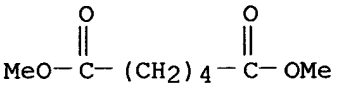
CRN 624-24-8
CMF C6 H12 O2



14 REFERENCES IN FILE CA (1962 TO DATE)
14 REFERENCES IN FILE CAPLUS (1962 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d que l5;d l5
L5 2 SEA FILE=REGISTRY ABB=ON PLU=ON "METHYL ADIPATE"/CN

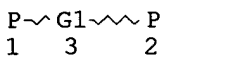
L5 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2003 ACS
RN 627-93-0 REGISTRY
CN Hexanedioic acid, dimethyl ester (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Adipic acid, dimethyl ester (6CI, 8CI)
OTHER NAMES:
CN DBE 6
CN Dimethyl adipate
CN Dimethyl hexanedioate
CN **Methyl adipate**
FS 3D CONCORD
DR 111366-61-1
MF C8 H14 O4
CI COM
LC STN Files: ANABSTR, AQUIRE, BEILSTEIN*, BIOSIS, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DETHERM*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MSDS-OHS, NIOSHTIC, PIRA, PROMT, RTECS*, SPECINFO, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1034 REFERENCES IN FILE CA (1962 TO DATE)
45 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1033 REFERENCES IN FILE CAPLUS (1962 TO DATE)
49 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d que stat l8
L6 STR



phosphorus - catalyst

REP G1=(1-4) A
NODE ATTRIBUTES:
NSPEC IS R AT 1
NSPEC IS R AT 2
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE
L7 SCR 2017 AND 1839
L8 3282 SEA FILE=REGISTRY SSS FUL L6 AND L7

100.0% PROCESSED 348897 ITERATIONS (1 INCOMPLETE) 3282 ANSWERS
SEARCH TIME: 00.00.03

=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 08:33:18 ON 17 APR 2003
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FILE COVERS 1907 - 17 Apr 2003 VOL 138 ISS 16
FILE LAST UPDATED: 16 Apr 2003 (20030416/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d his l9-

(FILE 'REGISTRY' ENTERED AT 08:18:37 ON 17 APR 2003)

FILE 'HCAPLUS' ENTERED AT 08:28:01 ON 17 APR 2003

FILE 'REGISTRY' ENTERED AT 08:28:10 ON 17 APR 2003
E CARBON MONOXIDE/CN
L9 1 S E3

FILE 'HCAPLUS' ENTERED AT 08:28:18 ON 17 APR 2003
L10 119149 S L1 OR BUTADIENE
L11 703 S DIENE# (L) CARBONYL?
L12 1491 S L8
L13 22 S L10 AND L12
L14 4 S L11 AND L12
L15 22 S L14 OR L13
L16 1374 S L4 OR L5
L17 119687 S L10 OR L11
L18 64 S L17 AND L16
L19 35 S L18 AND (CATALY? OR CAT/RL)
L20 20 S L19 AND CARBONYL?
L21 260284 S L9 OR CARBON DIOXIDE#
L22 21 S L21 AND L19
L23 13 S L22 AND L20
L24 10 S L23 NOT L15
L25 1 S L24 AND (P OR PHOSPHOR? OR PHOSPHOR?/AB)

FILE 'REGISTRY' ENTERED AT 08:32:15 ON 17 APR 2003

FILE 'HCAPLUS' ENTERED AT 08:33:18 ON 17 APR 2003

=> d .ca hitstr l15 1-22; d.ca hitstr l25 1

L15 ANSWER 1 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2003:58044 HCAPLUS
DOCUMENT NUMBER: 138:107148
TITLE: Process and catalyst system for the **carbonylation** of a conjugated **diene** and use of this process in the preparation of caprolactam or adipic acid
INVENTOR(S): Drent, Eit; Van Broekhoven, Johannes Adrianus Maria; Breed, Anthonius Johannes Maria
PATENT ASSIGNEE(S): DSM N.V., Neth.
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003006416	A1	20030123	WO 2002-NL461	20020711

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: EP 2001-306055 A 20010713

OTHER SOURCE(S): MARPAT 138:107148

AB A process for the carbonylation of a conjugated diene (e.g., 1,3-butadiene) comprises reacting the conjugated diene with carbon monoxide and an alkanol (e.g., methanol) in the presence of a metal-based catalyst [e.g., palladium acetate with the diphosphine 1,2-bis(9-phosphabicyclononyl)ethane] to form an ester, a polymeric byproduct (e.g., polybutadiene) is formed, the polymeric byproduct is sepd. from the metal-based catalyst with help of a solvent (e.g., di-Me adipate). This process is be used in the prepn. of caprolactam or adipic acid and process flow diagrams are presented.

IC ICM C07C067-38
ICS C07C069-44; C07C069-533

CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 23, 48, 67

ST caprolactam adipic acid manuf **butadiene** carbonylation

IT Alcohols, reactions
RL: EPR (Engineering process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(aliph.; process and catalyst system for the **carbonylation** of a conjugated **diene** and use of this process in the prepn. of caprolactam or adipic acid using)

IT Alkadienes
RL: EPR (Engineering process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(conjugated; process and catalyst system for the **carbonylation** of a conjugated **diene** and use of this process in the prepn. of caprolactam or adipic acid)

IT Phosphines
RL: CAT (Catalyst use); EPR (Engineering process); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(diphosphines; in a catalyst system for the **carbonylation** of a conjugated **diene** and use of this process in the prepn. of caprolactam or adipic acid)

IT **Carbonylation**
(of a conjugated **diene** and use of this process in the prepn. of caprolactam or adipic acid)

IT 9003-17-2P, Polybutadiene
RL: BYP (Byproduct); EPR (Engineering process); PEP (Physical, engineering or chemical process); PREP (Preparation); PROC (Process)
(byproduct; process and catalyst system for the **carbonylation** of a conjugated **diene** and use of this process in the prepn. of caprolactam or adipic acid)

IT 3375-31-3
RL: CAT (Catalyst use); EPR (Engineering process); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(catalyst system for the **carbonylation** of a conjugated **diene** and use of this process in the prepn. of caprolactam or adipic acid)

IT **153280-11-6 374557-18-3**
RL: CAT (Catalyst use); EPR (Engineering process); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(catalyst system with Pd for the **carbonylation** of a conjugated **diene** and use of this process in the prepn. of caprolactam or adipic acid)

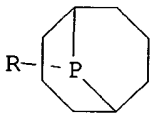
IT 105-60-2P, Caprolactam, preparation 124-04-9P, Adipic acid, preparation
RL: EPR (Engineering process); IMF (Industrial manufacture); PEP (Physical, engineering or chemical process); PREP (Preparation); PROC (Process)
(process and catalyst system for the **carbonylation** of a conjugated **diene** and use of this process in the prepn. of caprolactam or adipic acid)

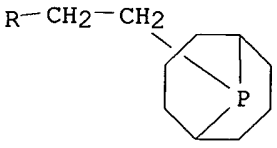
IT **106-99-0**, 1,3-**Butadiene**, reactions 630-08-0, Carbon monoxide, reactions
RL: EPR (Engineering process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(process and catalyst system for the **carbonylation** of a conjugated **diene** and use of this process in the prepn. of caprolactam or adipic acid)

IT 627-93-0, Dimethyl adipate
RL: EPR (Engineering process); NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(solvent; process and catalyst system for the **carbonylation** of a conjugated **diene** and use of this process in the prepn. of caprolactam or adipic acid)

IT **153280-11-6 374557-18-3**
RL: CAT (Catalyst use); EPR (Engineering process); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(catalyst system with Pd for the **carbonylation** of a conjugated **diene** and use of this process in the prepn. of caprolactam or adipic acid)

RN 153280-11-6 HCAPLUS
CN 9-Phosphabicyclo[3.3.1]nonane, 9,9'-(1,2-ethanediyl)bis- (9CI) (CA INDEX NAME)

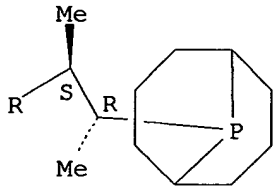


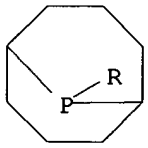


RN 374557-18-3 HCAPLUS

CN 9-Phosphabicyclo[3.3.1]nonane, 9,9'-[(1R,2S)-1,2-dimethyl-1,2-ethanediyl]bis-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.





IT **106-99-0**, 1,3-**Butadiene**, reactions
RL: EPR (Engineering process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(process and catalyst system for the **carbonylation** of a conjugated **diene** and use of this process in the prepn. of caprolactam or adipic acid)
RN 106-99-0 HCAPLUS
CN 1,3-Butadiene (8CI, 9CI) (CA INDEX NAME)

$H_2C{=}CH{-}CH{=}CH_2$

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:811991 HCAPLUS
DOCUMENT NUMBER: 137:325772
TITLE: Preparation of epsilon-caprolactam from **butadiene**
INVENTOR(S): Smits, Hubertus Adrianus; Sielcken, Otto; Haasen, Nicolaas Franciscus; Guit, Rudolf Philippus Maria; Tinge, Johan Thomas
PATENT ASSIGNEE(S): DSM N.V., Neth.
SOURCE: Eur. Pat. Appl., 21 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1251122	A1	20021023	EP 2001-201356	20010417
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
WO 2002083635 A1 20021024 WO 2002-NL250 20020417
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.: EP 2001-201356 A 20010417

AB The prepn. of .epsilon.-caprolactam starting from butadiene, CO, H and NH3, comprises (1) carbonylating butadiene in the presence of an alkanol and a catalyst comprising Pd, a multidentate phosphine ligand and an acidic co-catalyst to produce alkyl-4-, alkyl-3- and alkyl-2-pentenoate, optionally isomerizing the alkyl-3- and/or alkyl-2-pentenoate into alkyl-4-pentenoate, (2) hydroformylating the alkyl-4-, alkyl-3- and alkyl-2-pentenoate in the presence of a catalyst comprising Rh and an org. phosphorus-contg. ligand to produce alkyl-5-formyl valerate, (3) reductively aminating alkyl-5-formyl valerate in the presence of a hydrogenation catalyst comprising Ru on a carrier catalyst to produce .epsilon.-caprolactam and .epsilon.-caprolactam precursors, and (4) optionally, converting .epsilon.-caprolactam precursors at elevated temp. into .epsilon.-caprolactam.

IC ICM C07D201-08
CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 67
ST caprolactam manuf **butadiene** carbonylation hydroformylation reductive amination

IT Amination catalysts
(reductive; three step prepn. of epsilon-caprolactam from **butadiene** to high conversion without formation of ammonium sulfate byproduct)

IT Carbonylation catalysts
Hydrogenation catalysts
(three step prepn. of epsilon-caprolactam from **butadiene** to high conversion without formation of ammonium sulfate byproduct)

IT **473440-90-3 473440-91-4 473440-92-5 473440-93-6 473440-94-7**
RL: CAT (Catalyst use); USES (Uses)
(carbonylation catalyst; in Me pentenoate hydroformylation to Me formyl valerate)

IT 7440-05-3, Palladium, uses 14874-82-9, Rhodium biscarbonyl acetylacetonate **297731-74-9**
RL: CAT (Catalyst use); USES (Uses)
(carbonylation catalyst; three step prepn. of epsilon-caprolactam from **butadiene** to high conversion without formation of ammonium sulfate byproduct)

IT 6654-36-0P, Methyl 5-formyl valerate
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(intermediate hydroformylation; three step prepn. of epsilon-caprolactam from **butadiene** to high conversion without formation of ammonium sulfate byproduct)

IT 818-58-6, Methyl 3-pentenoate
RL: RCT (Reactant); RACT (Reactant or reagent)

(intermediate hydroformylation; three step prepn. of epsilon-caprolactam from **butadiene** to high conversion without formation of ammonium sulfate byproduct)

IT 196299-56-6
RL: CAT (Catalyst use); USES (Uses)
(ligand; three step prepn. of epsilon-caprolactam from **butadiene** to high conversion without formation of ammonium sulfate byproduct)

IT 7440-02-0, Nickel, uses 7440-18-8, Ruthenium, uses
RL: CAT (Catalyst use); USES (Uses)
(reductive amination catalyst; three step prepn. of epsilon-caprolactam from **butadiene** to high conversion without formation of ammonium sulfate byproduct)

IT **106-99-0, Butadiene,** reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting materials; three step prepn. of epsilon-caprolactam from **butadiene** to high conversion without formation of ammonium sulfate byproduct)

IT 1344-28-1, Alumina, uses 13463-67-7, Titania, uses
RL: CAT (Catalyst use); USES (Uses)
(support; three step prepn. of epsilon-caprolactam from **butadiene** to high conversion without formation of ammonium sulfate byproduct)

IT 6163-58-2, Tri-2-tolyl phosphine
RL: CAT (Catalyst use); USES (Uses)
(three step prepn. of epsilon-caprolactam from **butadiene** to high conversion without formation of ammonium sulfate byproduct)

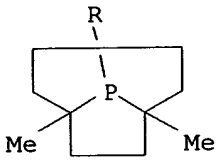
IT 105-60-2P, .epsilon.-Caprolactam, preparation
RL: IMF (Industrial manufacture); PUR (Purification or recovery); PREP (Preparation)
(three step prepn. of epsilon-caprolactam from **butadiene** to high conversion without formation of ammonium sulfate byproduct)

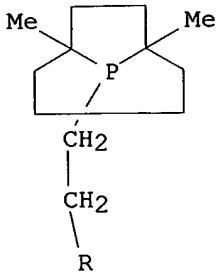
IT 7664-41-7, Ammonia, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(three step prepn. of epsilon-caprolactam from **butadiene** to high conversion without formation of ammonium sulfate byproduct)

IT 627-91-8, Monomethyl adipate
RL: CAT (Catalyst use); USES (Uses)
(weak acid; three step prepn. of epsilon-caprolactam from **butadiene** to high conversion without formation of ammonium sulfate byproduct)

IT **473440-90-3 473440-91-4 473440-92-5 473440-93-6 473440-94-7**
RL: CAT (Catalyst use); USES (Uses)
(carbonylation catalyst; in Me pentenoate hydroformylation to Me formyl valerate)

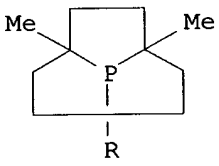
RN 473440-90-3 HCAPLUS
CN 9-Phosphabicyclo[4.2.1]nonane, 9,9'-(1,2-ethanediyl)bis[1,6-dimethyl- (9CI) (CA INDEX NAME)

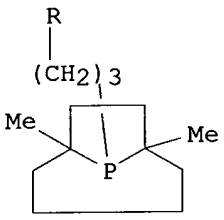




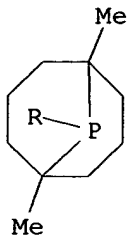
RN 473440-91-4 HCAPLUS
CN 9-Phosphabicyclo[3.3.1]nonane, 9,9'-(1,3-propanediyl)bis[1,5-dimethyl-(9CI) (CA INDEX NAME)

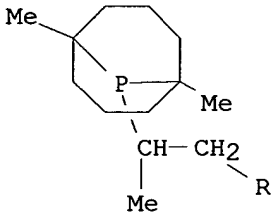
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 473440-92-5 HCAPLUS
CN 9-Phosphabicyclo[4.2.1]nonane, 9,9'-(1,3-propanediyl)bis[1,6-dimethyl-(9CI) (CA INDEX NAME)





RN 473440-93-6 HCAPLUS
CN 9-Phosphabicyclo[3.3.1]nonane, 9,9'-(1-methyl-1,2-ethanediyl)bis[1,5-dimethyl- (9CI) (CA INDEX NAME)





RN 473440-94-7 HCAPLUS
CN 9-Phosphabicyclo[4.2.1]nonane, 9,9'-(1-methyl-1,2-ethanediyl)bis[1,6-dimethyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
IT **297731-74-9**
RL: CAT (Catalyst use); USES (Uses)
(carbonylation catalyst; three step prepn. of epsilon-caprolactam from **butadiene** to high conversion without formation of ammonium sulfate byproduct)
RN 297731-74-9 HCAPLUS
CN 9-Phosphabicyclo[3.3.1]nonane, 9,9'-(1,2-ethanediyl)bis[1,5-dimethyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
IT **106-99-0, Butadiene,** reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting materials; three step prepn. of epsilon-caprolactam from **butadiene** to high conversion without formation of ammonium sulfate byproduct)
RN 106-99-0 HCAPLUS
CN 1,3-Butadiene (8CI, 9CI) (CA INDEX NAME)

$H_2C{=}CH{-}CH{=}CH_2$

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:256216 HCAPLUS
DOCUMENT NUMBER: 136:296537
TITLE: Process and palladium-diphosphine catalyst system for the **carbonylation** of conjugated **dienes**

Hector Reyes 09/937,122

INVENTOR(S): Drent, Eit; Jager, Willem Wabe; Sielcken, Otto Erik; Toth, Imre

PATENT ASSIGNEE(S): DSM N.V., Neth.

SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002026690	A1	20020404	WO 2001-NL709	20010926
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002011067	A5	20020408	AU 2002-11067	20010926

PRIORITY APPLN. INFO.:
EP 2000-203355 A 20000927
EP 2000-203356 A 20000927
EP 2000-2000203355A 20000927
EP 2000-2000203356A 20000927
WO 2001-NL709 W 20010926

OTHER SOURCE(S): MARPAT 136:296537

AB Conjugated dienes (e.g., 1,3-butadiene) are readily subjected to carbonylation to produce unsatd. esters (e.g., Me 3-pentenoate which is an adipate ester precursor) by reacting the conjugated diene with carbon monoxide and an hydroxyl group-contg. compd. (e.g., methanol) in the presence of a catalyst system based on: (a) a source of palladium cations (e.g., palladium acetate); (b) a diphosphine ligand X1RX2 (X1, X2 = cyclic group with at least 5 ring atoms of which one is a phosphorus atom; R = bivalent aliph. bridging group, connecting both phosphorus atoms contg. from 2 to 4 atoms in the bridge which is substituted with at least one substituent, Ph group with both phosphorus groups bound to the 1,2-position); and (c) a source of anions (e.g., pivalic acid).

IC ICM C07C067-38
ICS B01J031-28; B01J031-24

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23, 48, 67

ST conjugated **diene carbonylation** catalyst system; unsatd ester manuf conjugated **diene carbonylation**; palladium diphosphine catalyst conjugated **diene carbonylation**

IT **Carbonylation** catalysts
(Pd and diphosphine ligands and a source of anions for the conversion of conjugated **dienes** with alcs. into unsatd. carboxylate esters)

IT Alcohols, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(aliph.; process and palladium-diphosphine catalyst system for the **carbonylation** of conjugated **dienes** in the presence of)

IT Alkadienes
RL: RCT (Reactant); RACT (Reactant or reagent)

(conjugated; process and catalyst system for the **carbonylation** of conjugated **dienes**)

IT Phosphines
RL: CAT (Catalyst use); USES (Uses)
(diphosphines; ligands in a **carbonylation** catalyst system for the **carbonylation** of conjugated **dienes**)

IT **Carbonylation**
(of conjugated **dienes** with alcs. into unsatd. carboxylate esters)

IT Glycols, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(process and palladium-diphosphine catalyst system for the **carbonylation** of conjugated **dienes** in the presence of)

IT Carboxylic acids, uses
RL: CAT (Catalyst use); USES (Uses)
(tertiary; catalysts with palladium-diphosphine complex for the **carbonylation** of conjugated **dienes**)

IT Esters, preparation
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(unsatd.; process and palladium-diphosphine catalyst system for the **carbonylation** of conjugated **dienes** into)

IT 75-98-9, Pivalic acid 3375-31-3 7440-05-3, Palladium, uses
10034-85-2, Hydrogen iodide 52627-73-3, Versatic-10 **374557-18-3**
407578-79-4
RL: CAT (Catalyst use); USES (Uses)
(process and palladium-diphosphine catalyst system for the **carbonylation** of conjugated **dienes**)

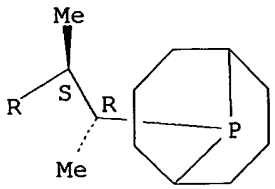
IT 67-56-1, Methanol, reactions **106-99-0**, 1,3-**Butadiene**, reactions 630-08-0, Carbon monoxide, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(process and palladium-diphosphine catalyst system for the **carbonylation** of conjugated **dienes**)

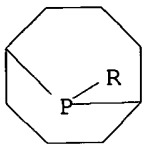
IT 818-57-5P, Methyl 4-pentenoate 818-58-6P, Methyl 3-pentenoate
818-59-7P, Methyl 2-pentenoate
RL: SPN (Synthetic preparation); PREP (Preparation)
(process and palladium-diphosphine catalyst system for the **carbonylation** of conjugated **dienes**)

IT **374557-18-3**
RL: CAT (Catalyst use); USES (Uses)
(process and palladium-diphosphine catalyst system for the **carbonylation** of conjugated **dienes**)

RN 374557-18-3 HCAPLUS
CN 9-Phosphabicyclo[3.3.1]nonane, 9,9'-[(1R,2S)-1,2-dimethyl-1,2-ethanediyl]bis-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.





IT **106-99-0**, 1,3-**Butadiene**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(process and palladium-diphosphine catalyst system for the **carbonylation** of conjugated **dienes**)
RN 106-99-0 HCAPLUS
CN 1,3-Butadiene (8CI, 9CI) (CA INDEX NAME)

$H_2C{=}CH{-}CH{=}CH_2$

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:847401 HCAPLUS
DOCUMENT NUMBER: 136:8065
TITLE: Production method of organophosphorus fire-retarding agents
INVENTOR(S): Sumitomo, Hiroshi; Hirayama, Takumi; Ikemoto, Kenichi; Saito, Toranosuke
PATENT ASSIGNEE(S): Sanko Co., Inc., Japan; Saito Kaseihin Kenkysho Y. K.
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001323268	A2	20011122	JP 2000-143816	20000516

PRIORITY APPLN. INFO.: JP 2000-143816 20000516
OTHER SOURCE(S): MARPAT 136:8065
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Organophosphorus compd. represented by (I), wherein R1 and R2 = H or lower alkyl, Y and X1-8 = H, alkyl, cycloalkyl, aryl, or aralkyl, and n = 1-3 is obtained by reacting organophosphorus compd. (II), aldehydes or ketones and ammonia or condensation products of organo-primary amine or organo secondary amines. Fire-retardant materials comprise 100 parts resins and 5-35 parts I. Thus, 540 g 9,10-dihydro-9-oxa-10-phosphaphenanthrene 10-oxide and 58.3 g hexamethylene tetramine were heated at 170.degree. for 1 h to give (III). To Techno Polymer 170 (acrylonitrile-butadiene-styrene copolymer) 5% organophosphorus was added, kneaded to give pellets, and extruded to give a test-piece showing fire-retardancy (UL 94) V-2.

IC ICM C09K021-12
ICS C07F009-6574; C08K005-5313; C08L101-00

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 38

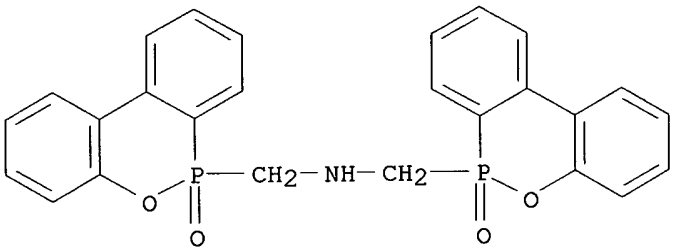
IT 9003-56-9, Acrylonitrile-**butadiene**-styrene copolymer
RL: TEM (Technical or engineered material use); USES (Uses)
(Technopolymer 170; prodn. method of organophosphorus fire-retarding agents)

IT **106871-32-3P 374793-64-3P** 374793-66-5P
RL: IMF (Industrial manufacture); PREP (Preparation)
(prodn. method of organophosphorus fire-retarding agents)

IT **106871-32-3P 374793-64-3P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(prodn. method of organophosphorus fire-retarding agents)

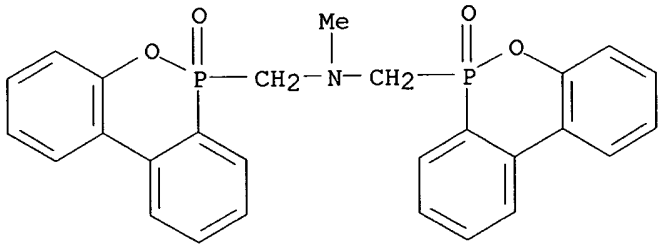
RN 106871-32-3 HCAPLUS

CN 6H-Dibenz[c,e][1,2]oxaphosphorin-6-methanamine, N-[(6-oxido-6H-dibenz[c,e][1,2]oxaphosphorin-6-yl)methyl]-, 6-oxide (9CI) (CA INDEX NAME)



RN 374793-64-3 HCAPLUS

CN 6H-Dibenzo[c,e][1,2]oxaphosphorin-6-methanamine, N-methyl-N-[(6-oxido-6H-dibenzo[c,e][1,2]oxaphosphorin-6-yl)methyl]-, 6-oxide (9CI) (CA INDEX NAME)



L15 ANSWER 5 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:165772 HCAPLUS
DOCUMENT NUMBER: 134:208685
TITLE: Flame-retardant polycarbonate blends and their use
INVENTOR(S): Zobel, Michael; Eckel, Thomas; Derr, Torsten; Wittmann, Dieter
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 14 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19941822	A1	20010308	DE 1999-19941822	19990902
WO 2001018120	A1	20010315	WO 2000-EP8169	20000822
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000013726	A	20020507	BR 2000-13726	20000822
EP 1214379	A1	20020619	EP 2000-956474	20000822
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003509526	T2	20030311	JP 2001-522336	20000822

PRIORITY APPLN. INFO.: DE 1999-19941822 A 19990902
WO 2000-EP8169 W 20000822

OTHER SOURCE(S): MARPAT 134:208685

AB Fire-retardant blends contain arom. polycarbonate and/or polyester carbonate 40-99, special graft polymers manufd. by means of redox initiator systems 0.5-60, thermoplastic(s) 0-45, fluorinated polyolefin 0-5, and an aminomethylphosphonate of the type A3-yNXy, where A is 5,5-disubstituted 1,3,2-dioxaphosphorinanylmethyl or (RO)(R1O)P(O)CH2 (R, R1 = optionally substituted alkyl or aryl; RR1 may form alkylene), X = H, optionally halogenated C2-8-alkyl, or C6-10-aryl, and y = 0, 1, or 2 0.1-30 parts and have good mech. properties. An example contained bisphenol A polycarbonate, ABS graft copolymer prepd. using cumene hydroperoxide and ascorbic acid, SAN polymer, PTFE, and XPM 1000 fire retardant.

IC ICM C08L069-00
ICS C08L051-04; C08K005-5317; C08K005-5357; C09K021-14

CC 37-6 (Plastics Manufacture and Processing)

IT **Butadiene** rubber, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(graft polymn. of)

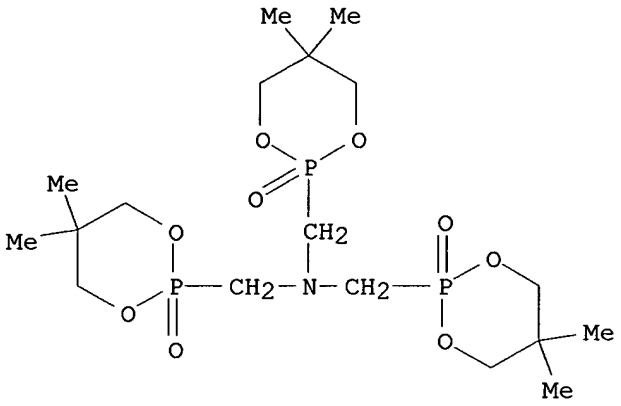
IT 9003-17-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(**butadiene** rubber, graft polymn. of)

IT **154704-76-4**, XPM 1000 **216699-57-9 329033-27-4**

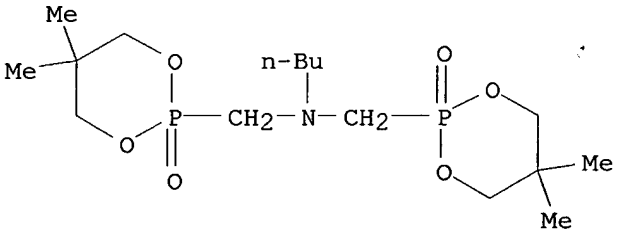
329033-28-5 **329033-29-6 329033-30-9**
329033-31-0 329033-32-1 **329033-33-2**
RL: MOA (Modifier or additive use); USES (Uses)
(fireproofing agent; flame-retardant polycarbonate molding materials contg.)

IT **154704-76-4,** XPM 1000 **216699-57-9 329033-27-4**
329033-29-6 329033-30-9 329033-31-0
329033-33-2
RL: MOA (Modifier or additive use); USES (Uses)
(fireproofing agent; flame-retardant polycarbonate molding materials contg.)

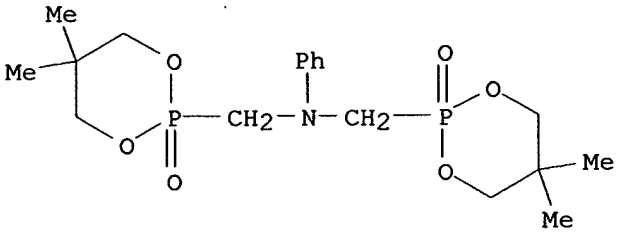
RN 154704-76-4 HCAPLUS
CN 1,3,2-Dioxaphosphorinane-2-methanamine, N,N-bis[(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)methyl]-5,5-dimethyl-, 2-oxide (9CI) (CA INDEX NAME)



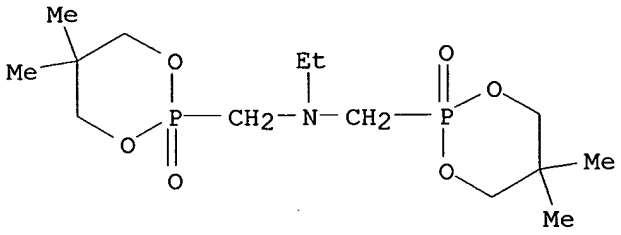
RN 216699-57-9 HCAPLUS
CN 1,3,2-Dioxaphosphorinane-2-methanamine, N-butyl-N-[(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)methyl]-5,5-dimethyl-, 2-oxide (9CI) (CA INDEX NAME)



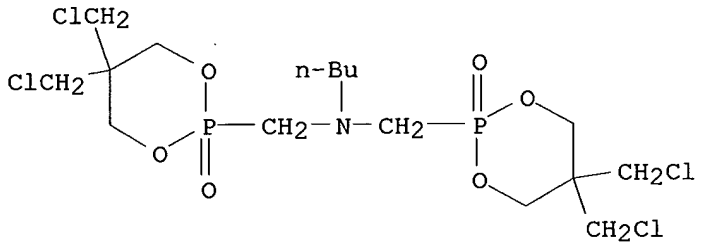
RN 329033-27-4 HCAPLUS
CN 1,3,2-Dioxaphosphorinane-2-methanamine, N-[(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)methyl]-5,5-dimethyl-N-phenyl-, 2-oxide (9CI) (CA INDEX NAME)



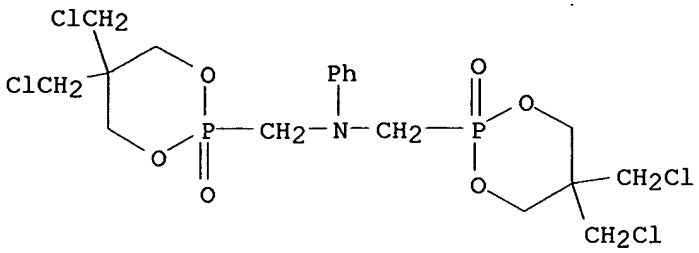
RN 329033-29-6 HCAPLUS
CN 1,3,2-Dioxaphosphorinane-2-methanamine, N-[(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)methyl]-N-ethyl-5,5-dimethyl-, 2-oxide (9CI) (CA INDEX NAME)



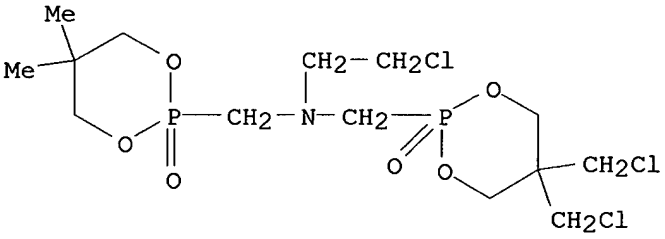
RN 329033-30-9 HCAPLUS
CN 1,3,2-Dioxaphosphorinane-2-methanamine, N-[[5,5-bis(chloromethyl)-2-oxido-1,3,2-dioxaphosphorinan-2-yl]methyl]-N-butyl-5,5-bis(chloromethyl)-, 2-oxide (9CI) (CA INDEX NAME)



RN 329033-31-0 HCAPLUS
CN 1,3,2-Dioxaphosphorinane-2-methanamine, N-[[5,5-bis(chloromethyl)-2-oxido-1,3,2-dioxaphosphorinan-2-yl]methyl]-5,5-bis(chloromethyl)-N-phenyl-, 2-oxide (9CI) (CA INDEX NAME)



RN 329033-33-2 HCAPLUS
CN 1,3,2-Dioxaphosphorinane-2-methanamine, N-[[5,5-bis(chloromethyl)-2-oxido-1,3,2-dioxaphosphorinan-2-yl]methyl]-N-(2-chloroethyl)-5,5-dimethyl-, 2-oxide (9CI) (CA INDEX NAME)



L15 ANSWER 6 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:688203 HCAPLUS
DOCUMENT NUMBER: 133:268554
TITLE: Process for the **carbonylation** of conjugated **dienes**
INVENTOR(S): Drent, Eit; Jager, Willem Wabe
PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B.V., Neth.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000056695	A1	20000928	WO 2000-EP2375	20000316
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1163202	A1	20011219	EP 2000-910854	20000316
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

BR 2000009187	A	20011226	BR 2000-9187	20000316
JP 2002540091	T2	20021126	JP 2000-606559	20000316

PRIORITY APPLN. INFO.: EP 1999-302202 A 19990322
WO 2000-EP2375 W 20000316

AB The present invention relates to a process for the carbonylation of conjugated dienes, whereby a conjugated diene is reacted with carbon monoxide and a hydroxyl group contg. compd. in the presence of a catalyst system including: (a) a source of palladium cations, (b) a phosphorus-contg. ligand, (c) a source of anions, wherein the phosphorus-contg. ligand is a ligand having the general formula X1-R-X2 wherein X1 and X2 represent a substituted or non-substituted cyclic group with at least 5 ring atoms, of which one is a phosphorus atom, and R represents a bivalent org. bridging group, connecting both phosphorus atoms, contg. from 1 to 4 atoms in the bridge, whereby the carbonylation process can be performed batch wise, semi-continuously or continuously. Thus, a mixt. of 40 mL methanol, 40 mL anisole, 0.5 mmol palladium acetate, 0.6 mmol 1,2-P,P'-bis(9-phosphabicyclononyl)ethane, 2 mmol 2,6-dimethoxybenzoic acid, 20 mL 1,3-butadiene, and CO to an initial CO pressure of 40 bar was heated to 170.degree. and reacted for 10 h to give carbonylation products with >95% total selectivity.

IC ICM C07C067-38
ICS C07C069-533; C07C069-44; B01J031-24

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)

ST **butadiene** carbonylation catalyst palladium phosphorus ligand; dimethoxybenzoic acid **butadiene** carbonylation catalyst palladium phosphorus

IT Carbonylation catalysts
(carbonylation of **butadiene** in presence of palladium-phosphorus compd.)

IT 627-93-0P, Dimethyl adipate 14035-94-0P 14035-95-1P 69665-13-0P, Dimethyl propylmaleate
RL: IMF (Industrial manufacture); PREP (Preparation)
(carbonylation of **butadiene** in presence of palladium-phosphorus compd.)

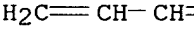
IT **106-99-0**, 1,3-**Butadiene**, reactions 630-08-0, Carbon monoxide, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(carbonylation of **butadiene** in presence of palladium-phosphorus compd.)

IT 480-63-7 1466-76-8 3375-31-3, Palladium diacetate 5204-64-8, 3-Pentenoic acid **153280-11-6 297731-74-9**
RL: CAT (Catalyst use); USES (Uses)
(catalysts; carbonylation of **butadiene** in presence of palladium-phosphorus compd.)

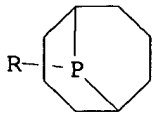
IT 259110-39-9
RL: CAT (Catalyst use); USES (Uses)
(catalysts; g r6carbonylation of **butadiene** in presence of palladium-phosphorus compd.)

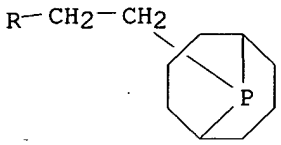
IT **106-99-0**, 1,3-**Butadiene**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(carbonylation of **butadiene** in presence of palladium-phosphorus compd.)

RN 106-99-0 HCAPLUS
CN 1,3-Butadiene (8CI, 9CI) (CA INDEX NAME)



IT **153280-11-6 297731-74-9**
RL: CAT (Catalyst use); USES (Uses)
(catalysts; carbonylation of **butadiene** in presence of palladium-phosphorus compd.)
RN 153280-11-6 HCAPLUS
CN 9-Phosphabicyclo[3.3.1]nonane, 9,9'-(1,2-ethanediyl)bis- (9CI) (CA INDEX NAME)





RN 297731-74-9 HCAPLUS
CN 9-Phosphabicyclo[3.3.1]nonane, 9,9'-(1,2-ethanediyl)bis[1,5-dimethyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 7 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:409658 HCAPLUS
DOCUMENT NUMBER: 131:152997
TITLE: From a terminal (cis-2-butene-1,4-diyl-1,4-diphosphinidene) complex to some new diphosphorus bicycles
AUTHOR(S): Hoa Tran Huy, Ngoc; Ricard, Louis; Mathey, Francois
CORPORATE SOURCE: Laboratoire Heteroelements et Coordination, DCPH, UMR 7653 CNRS, Ecole Polytechnique, Palaiseau, F-91128, Fr.
SOURCE: Journal of Organometallic Chemistry (1999), 582(1), 53-57
CODEN: JORCAI; ISSN: 0022-328X
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The reaction of the transient [cis-2-butene-1,4-diyl-1,4-diphosphinidene]decacarbonylditungsten complex (3) as generated from the appropriate 7-phosphanorbornadiene precursor (2) at 60.degree. in the presence of CuCl as a catalyst with 3-hexyne, 2,3-dimethylbutadiene and [phenyl(methoxy)carbene]pentacarbonyltungsten yields the products [7,8-diethyl-1,6-diphosphabicyclo[4.2.0]octa-3,7-diene]decacarbonylditungsten (5), [3,4-dimethyl-1,6-diphosphabicyclo[4.4.0]deca-3,8-diene]decacarbonylditungsten (7) and [7-methoxy-7-phenyl-1,6-diphosphabicyclo[4.1.0]hept-3-ene]decacarbonylditungsten (8). These products formally result from the

[2+2], [4+2] and [1+2] cycloaddns. of the reagents with the P:P double bond of the [3,6-dihydro-1,2-diphosphinine]decacarbonylditungsten. However, a mechanism involving a monocondensation of the reagent onto one P of the bis-phosphinidene, followed by the insertion of the 2nd P into the monophosphorus heterocycles thus formed is favored.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 75

IT 513-81-5, 2,3-Dimethyl-1,3-**butadiene**
RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of tungsten bis(phosphiranyl)butene and diphosphabicyclodecadiene carbonyl dinuclear complexes)

IT **235114-63-3P 235114-65-5P** 235114-66-6P 235114-67-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and NMR of)

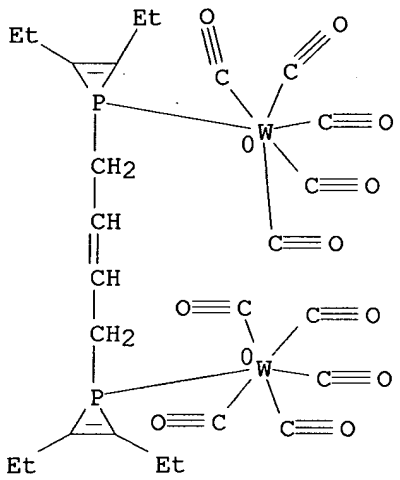
IT **235114-61-1P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn., NMR and cycloaddn. of acetylenedicarboxylic acid ester)

IT **235114-62-2P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn., NMR and reactions with hexyne, dimethylbutadiene and tungsten carbonyl carbene complex)

IT **235114-63-3P 235114-65-5P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and NMR of)

RN 235114-63-3 HCAPLUS

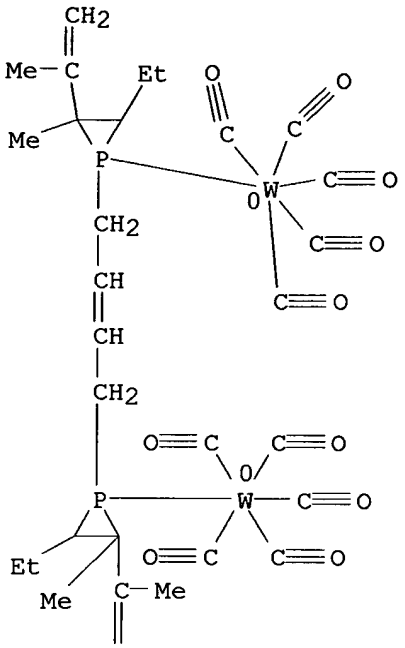
CN Tungsten, [.mu.-[1,1'-(2Z)-2-butene-1,4-diylbis[2,3-diethyl-1H-phosphirene-.kappa.P]]]decacarbonyldi- (9CI) (CA INDEX NAME)



RN 235114-65-5 HCAPLUS

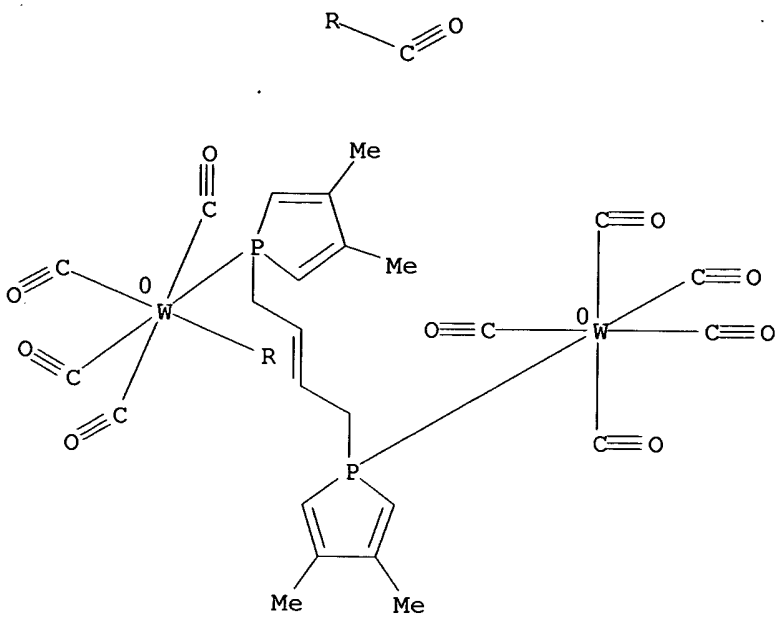
CN Tungsten, [.mu.-[1,1'-(2-butene-1,4-diyl)bis[3-ethyl-2-methyl-2-(1-methylethenyl)phosphirane-.kappa.P]]]decacarbonyldi- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

IT **235114-61-1P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn., NMR and cycloaddn. of acetylenedicarboxylic acid ester)
RN 235114-61-1 HCAPLUS
CN Tungsten, [.mu.-[1,1'-(2Z)-2-butene-1,4-diylbis[3,4-dimethyl-1H-phosphole-.kappa.P]]]decacarbonyldi- (9CI) (CA INDEX NAME)



IT **235114-62-2P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn., NMR and reactions with hexyne, dimethylbutadiene and tungsten carbonyl carbene complex)
RN 235114-62-2 HCAPLUS
CN Tungsten, decacarbonyl[.mu.-[tetramethyl (1R,1'R,4S,4'S)-7,7'-(2Z)-2-butene-1,4-diylbis[5,6-dimethyl-7-phosphabicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxylate-.kappa.P7]]]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 8 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:703454 HCAPLUS
DOCUMENT NUMBER: 129:317915
TITLE: Production of .epsilon.-caprolactones by carbonylation of penten-1-ols, catalysts therefor, and reaction mixtures therefrom
INVENTOR(S): Maher, John M.; Tjaden, Erik B.; Briggs, John R.; Guram, Anil S.
PATENT ASSIGNEE(S): Union Carbide Chemicals and Plastics Technology Corporation, USA
SOURCE: Eur. Pat. Appl., 47 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 872483	A1	19981021	EP 1998-302859	19980414

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

US 5883265 A 19990316 US 1997-834271 19970415

PRIORITY APPLN. INFO.: US 1997-834271 19970415

OTHER SOURCE(S): MARPAT 129:317915

AB (un)substituted .epsilon.-caprolactones and/or hydrates and/or esters thereof are prepd. by carbonylation of (un)substituted penten-1-ols in the presence of a carbonylation catalyst, e.g., a metal-organophosphorus ligand complex catalyst, and can undergo further reaction(s) to afford derivs., e.g., .epsilon.-caprolactam. The penten-1-ols are prepd. by hydroformylation of alkadienes to pentenals then hydrodenation of the pentenals, or directly by reductive hydroformylation of alkadienes. Thus, butadiene was reacted in the presence of dicarbonylacetylacetonatorhodium(I) and triethylphosphine at 300/300 psi H/CO and 80.degree. to give 90% butadiene conversion with 87% selectivity to 3- and 4-pentenols. A reactor contg. 0.18 mmol bis(triphenylphosphine)palladium(II) dichloride, 0.87 mmol SnCl2, 3 mL 4-pentenol, 26 mL MIBK, and 1 mL diglyme was pressured with 1600 psi CO at 100.degree. for 2.5 h with 77% 4-pentenol conversion, giving a mixt. of 3-pentenol 10, 2-ethylbutyrolactone 12, 2-methylvalerolactone 18, .epsilon.-caprolactone 49, and 3- and 4-pentenyl-6-hydroxyhexanoate 11%.

IC ICM C07D313-04
ICS C07C051-14

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 27

ST caprolactone prepn carbonylation pentenol; carbonylation catalyst metal organophosphorus ligand complex; palladium phenylphosphine catalyst carbonylation pentenol; phosphine ligand carbonylation catalyst; **butadiene** hydroformylation pentenol prepn

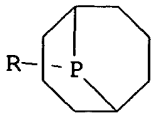
IT 554-70-1, Triethylphosphine 594-09-2, Trimethylphosphine 607-01-2, Ethyldiphenylphosphine 998-40-3, Tributylphosphine 1605-53-4, Diethylphenylphosphine 3375-31-3, Palladium diacetate 4706-17-6, Tris(3-hydroxypropyl)phosphine 4731-53-7, Trioctylphosphine 7772-99-8, Tin dichloride, uses 10210-68-1, Dicobalt octacarbonyl 13965-03-2, Bis(triphenylphosphine)palladium(II) dichloride 14874-82-9, Dicarbonylacetylacetonatorhodium(I) 17005-57-1 19262-01-2 32376-20-8, tert-Butyldiethylphosphine 50420-43-4 111982-81-1 **153280-11-6** 191665-95-9
RL: CAT (Catalyst use); USES (Uses)
(catalyst; prodn. of .epsilon.-caprolactones by carbonylation of penten-1-ols, catalysts therefor, and reaction mixts. therefrom)

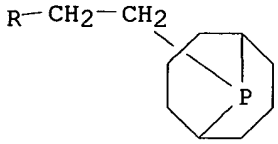
IT **106-99-0**, 1,3-**Butadiene**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(formylation to pentenols; prodn. of .epsilon.-caprolactones by carbonylation of penten-1-ols, catalysts therefor, and reaction mixts. therefrom)

IT **153280-11-6**
RL: CAT (Catalyst use); USES (Uses)
(catalyst; prodn. of .epsilon.-caprolactones by carbonylation of penten-1-ols, catalysts therefor, and reaction mixts. therefrom)

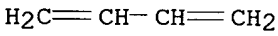
RN 153280-11-6 HCAPLUS

CN 9-Phosphabicyclo[3.3.1]nonane, 9,9'-(1,2-ethanediyl)bis- (9CI) (CA INDEX NAME)





IT **106-99-0**, 1,3-**Butadiene**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(formylation to pentenols; prodn. of .epsilon.-caprolactones by carbonylation of penten-1-ols, catalysts therefor, and reaction mixts. therefrom)
RN 106-99-0 HCAPLUS
CN 1,3-Butadiene (8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 9 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:703453 HCAPLUS
DOCUMENT NUMBER: 129:317914
TITLE: Production of .epsilon.-caprolactones and/or hydrates and/or esters thereof by carbonylation, catalysts therefor, and reaction mixtures therefrom
INVENTOR(S): Maher, John M.; Tjaden, Erik B.; Briggs, John R.; Guram, Anil S.
PATENT ASSIGNEE(S): Union Carbide Chemicals and Plastics Technology Corporation, USA
SOURCE: Eur. Pat. Appl., 30 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 872482	A2	19981021	EP 1998-302856	19980414
EP 872482	A3	19991006		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 6184391	B1	20010206	US 1997-839577	19970415
US 6307065	B1	20011023	US 2000-729408	20001204

PRIORITY APPLN. INFO.: US 1997-839577 A 19970415
OTHER SOURCE(S): MARPAT 129:317914
AB (Un)substituted .epsilon.-caprolactones and/or hydrates and/or esters

thereof are prepd. by hydrocarbonylation of (un)substituted alkadienes to (un)substituted penten-1-ols and carbonylation of the (un)substituted penten-1-ols in the presence of a carbonylation catalyst, e.g., a metal-organophosphorus ligand complex catalyst. The (un)substituted .epsilon.-caprolactones can undergo further reaction(s) to afford derivs., e.g., .epsilon.-caprolactam. Thus, butadiene was hydrocarbonylated in the presence of dicarbonylacetylacetonato rhodium(I) and triethylphosphine at 300/300 psi H/CO and 80.degree. to give 90% butadiene conversion with 87% selectivity to 3- and 4-pentenols. A reactor contg. 0.18 mmol bis(triphenylphosphine)palladium(II) dichloride, 0.87 mmol SnCl2, 3 mL 4-pentenol, 26 mL MIBK, and 1 mL diglyme was pressured with 1600 psi CO at 100.degree. for 2.5 h with 77% 4-pentenol conversion, giving 3-pentenol 10, 2-ethylbutyrolactone 12, 2-methylvalerolactone 18, .epsilon.-caprolactone 49, and 3- and 4-pentenyl-6-hydroxyhexanoate 11%.

IC ICM C07D313-04
ICS C07C067-38; C07C051-14

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 27, 35

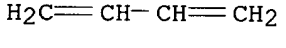
ST caprolactone prepn carbonylation pentenol; carbonylation catalyst metal organophosphorus ligand complex; palladium phenylphosphine catalyst carbonylation pentenol; phosphine ligand carbonylation catalyst; **butadiene** hydrocarbonylation pentenol prepn

IT **106-99-0**, 1,3-**Butadiene**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(carbonylation to pentenols; prodn. of .epsilon.-caprolactones and/or hydrates and/or esters thereof by carbonylation, catalysts therefor, and reaction mixts. therefrom)

IT 554-70-1, Triethylphosphine 594-09-2, Trimethylphosphine 607-01-2, Diphenylethylphosphine 998-40-3, Tributylphosphine 1605-53-4, Diethylphenylphosphine 3375-31-3, Palladium diacetate 4706-17-6, Tris(3-hydroxypropyl)phosphine 4731-53-7, Trioctylphosphine 7772-99-8, Tin dichloride, uses 10210-68-1, Dicobalt octacarbonyl 13965-03-2, Bis(triphenylphosphine)palladium(II) dichloride 14874-82-9, Dicarbonylacetylacetonatorhodium(I) 17005-57-1 19262-01-2 32376-20-8, tert-Butyldiethylphosphine 50420-43-4 111982-81-1 **153280-11-6** 173864-51-2
RL: CAT (Catalyst use); USES (Uses)
(catalyst; prodn. of .epsilon.-caprolactones and/or hydrates and/or esters thereof by carbonylation, catalysts therefor, and reaction mixts. therefrom)

IT **106-99-0**, 1,3-**Butadiene**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(carbonylation to pentenols; prodn. of .epsilon.-caprolactones and/or hydrates and/or esters thereof by carbonylation, catalysts therefor, and reaction mixts. therefrom)

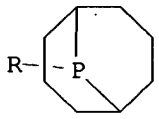
RN 106-99-0 HCAPLUS
CN 1,3-Butadiene (8CI, 9CI) (CA INDEX NAME)

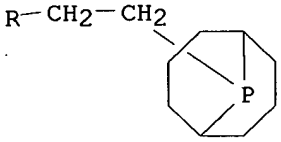


IT **153280-11-6**
RL: CAT (Catalyst use); USES (Uses)
(catalyst; prodn. of .epsilon.-caprolactones and/or hydrates and/or esters thereof by carbonylation, catalysts therefor, and reaction mixts. therefrom)

RN 153280-11-6 HCAPLUS

CN 9-Phosphabicyclo[3.3.1]nonane, 9,9'-(1,2-ethanediyl)bis- (9CI) (CA INDEX NAME)





L15 ANSWER 10 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:358077 HCAPLUS
DOCUMENT NUMBER: 129:136258
TITLE: Silylphosphine-alkene reaction routes to acyclic and cyclic organophosphines
AUTHOR(S): Schubert, David M.; Hackney, Michael L.; Brandt, Paul F.; Norman, Arlan D.
CORPORATE SOURCE: Dep. of Chemistry and Biochemistry, University of Colorado, Boulder, CO, 80309-0215, USA
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (1997), 123, 141-160
CODEN: PSSLEC; ISSN: 1042-6507
PUBLISHER: Gordon & Breach Science Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:136258

AB Radical reactions of Me3SiPH2, (Me3Si)2PH, Me2Si(PH2)2 and PH3 with selected alkanes have been exam. as routes to new organo(silyl)phosphines. The Me3SiPH2/1,5-hexadiene reaction initiated by AIBN yields the phosphepane Me3SiP(CH2)6 (11a) and acyclic Me3SiP[(CH2)4CH:CH2]2 (12); the Me3SiPH2/1,3-butadiene reaction yields only acyclic butenyl phosphines Me3SiP(H)C4H7 (14A-C) and Me3SiP(C4H7)2 (15A-D). Reactions of Me3SiPH2 with P(CH:CH2)3 and MeSi(CH:CH2)3 yield the vinyl-substituted cis- and trans-phosphorinanes (CH2:CH)P(C2H4)2PSiMe3 (18A/18B) and Me(CH2:CH)Si(C2H4)2PSiMe3 (20A/20B). (Me3Si)2PH/Me2Si(CH:CH2)2 reaction products only the acyclic (CH2:CH)Me2SiC2H4P(SiMe3)2 (22) and Me2Si[C2H4P(SiMe3)2]2 (25). The Me2Si(PH2)2/1,4-pentadiene reaction yields phosphorinanyl derivs. Me2Si(PH2)[P(CH2)5] (27) and Me2Si[P(CH2)5]2 (28); no large-ring products form. The AIBN initiated reaction of CH2:CHCH2PH2 has been reinvestigated; the known bicyclic [(CH2)3]2P2 is obtained instead of the previously reported tricyclic [(CH2)3]3P2. The PH3/Me2Si(CH:CH2)2 reaction yields mixts. of tentatively characterized Me2Si(C2H4)2PC2H4SiMe2(CH:CH2) (29) and [Me2Si(C2H4)2PC2H4]2SiMe2 (30). Solvolysis (with MeOH or H2O) of silylphosphines 11a, 27 (or 28), 12, 14A-C, 15A-D, 18A/18B, 20A/20B, 22 and 25 yields phosphorinanes (CH2)5PH (7) and Me2Si(C2H4)2PH (9), the new phosphenane (CH2)6PH (11b), HP[(CH2)4CH:CH2]2 (13), H2PC4H7 (16A-C), HP(C4H7)2 (17A-D), the cis- and trans-(CH2:CH)P(C2H4)2PH (19A/19B) and Me(CH2:CH)Si(C2H4)2PH (21A/21B),

(CH2:CH)Me2SiC2H4P(H)SiMe3 (23), (CH2:CH)Me2SiC2H4PH2 (24) and Me2Si(C2H4PH2)2 (26). Attempts to obtain new tricyclic or lage-ring cyclic phosphines by radical ring closure of 19A/19B and 21A/21B or cyclooligomerization of 23 or 24 were unsuccessful. New compds. are characterized by spectral (1H, 13C, and 31P NMR, MS and IR) data.

CC 29-7 (Organometallic and Organometalloidal Compounds)

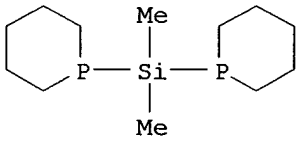
IT 6680-77-9P, Phosphepane 66872-86-4P 210412-25-2P 210412-28-5P
210412-30-9P 210412-34-3P 210412-35-4P **210412-36-5P**
210412-39-8P 210412-40-1P 210490-05-4P 210490-06-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **106-99-0**, 1,3-**Butadiene**, reactions 591-93-5, 1,4-Pentadiene 592-42-7, 1,5-Hexadiene 1113-12-8, Diallyldimethylsilane 3746-01-8, Trivinylphosphine 7803-51-2, Phosphine 10519-87-6, Dimethyldivinylsilane 15573-39-4, Bis(trimethylsilyl)phosphine 16523-89-0, Triallylphosphine 17446-52-5, (Trimethylsilyl)phosphine 18244-95-6, Methyltrivinylsilane 20519-91-9, Dimethyldiphosphinosilane 81637-99-2, Allylphosphine 124738-64-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(silylphosphine-alkene reaction routes to acyclic and cyclic organophosphines)

IT **210412-36-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 210412-36-5 HCAPLUS

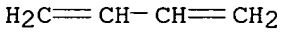
CN Phosphorinane, 1,1'-(dimethylsilylene)bis- (9CI) (CA INDEX NAME)



IT **106-99-0**, 1,3-**Butadiene**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(silylphosphine-alkene reaction routes to acyclic and cyclic organophosphines)

RN 106-99-0 HCAPLUS

CN 1,3-Butadiene (8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 11 OF 22 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:192481 HCAPLUS

DOCUMENT NUMBER: 126:271327

TITLE: Nickel(0) and palladium(0) complexes with 1,3,5-triaza-7-phosphaadamantane. Catalysis of buta-1,3-diene oligomerization or telomerization in an aqueous biphasic system

AUTHOR(S): Cermak, Jan; Kvicalova, Magdalena; Blechta, Vratislav

CORPORATE SOURCE: Inst. Chem. Process Fundamentals, Acad. Sci. Czech

Republic, Prague, 165 02, Czech Rep.
SOURCE: Collection of Czechoslovak Chemical Communications (1997), 62(2), 355-363
CODEN: CCCCAK; ISSN: 0010-0765
PUBLISHER: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
DOCUMENT TYPE: Journal
LANGUAGE: English

AB New homoleptic Ni(0) and Pd(0) complexes with a water-sol. ligand, 1,3,5-triaza-7-phosphaadamantane, were prepd. and characterized by 1H, 13P NMR spectra. The complexes, together with the known analogous Ni(0) and Pd(0) complexes with tris(hydroxymethyl)phosphine, are catalysts for buta-1,3-diene oligomerization or telomerization with H2O in an aq. biphasic system without a cosolvent or a modifier. Tetrakis[tris(hydroxymethyl)phosphine]nickel preferentially catalyzes oligomerization (both linear and cyclic) in the 1st example of a Ni-catalyzed buta-1,3-diene oligomerization in an aq. biphasic system. Pd complexes give telomers or linear oligomers in quant. yields. In the case of the triazaphosphaadamantane complex, high selectivity to octadienyl ethers (87%) was obsd. High values of metal leaching into the product phase in these reactions suggest an easy extn. of starting or intermediate metal complexes caused by the fact that both monomer and products are good ligands for the metal complexes in this particular case.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 2, 23, 67

ST triazaphosphaadamantane nickel palladium prepn oligomerization catalyst; telomerization catalyst palladium nickel triazaphosphaadamantane; **butadiene** oligomerization telomerization catalyst; hydroxymethylphosphine nickel palladium oligomerization telomerization catalyst

IT 125383-70-2
RL: CAT (Catalyst use); USES (Uses)
(catalyst in oligomerization and telomerization of **butadiene**)

IT **106-99-0**, Buta-1,3-diene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(oligomerization and telomerization in presence of nickel and palladium triazaphosphaadamantane/tris(hydroxymethyl)phosphine complex catalysts)

IT 125383-71-3P **188747-92-4P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(prepn. and catalysis in oligomerization and telomerization of **butadiene**)

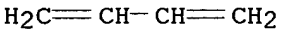
IT **188747-91-3P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(prepn. and lack of catalysis in oligomerization and telomerization of **butadiene**)

IT 766-03-0P, Vinyl-3-cyclohexene 3642-08-8P, 1,2,7-Octatriene 41233-05-0P, 1,2,6-Octatriene 86012-27-3P 188747-94-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. from oligomerization of **butadiene** in presence of nickel and palladium triazaphosphaadamantane/tris(hydroxymethyl)phosphine complex catalysts)

IT **106-99-0**, Buta-1,3-diene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(oligomerization and telomerization in presence of nickel and palladium triazaphosphaadamantane/tris(hydroxymethyl)phosphine complex catalysts)

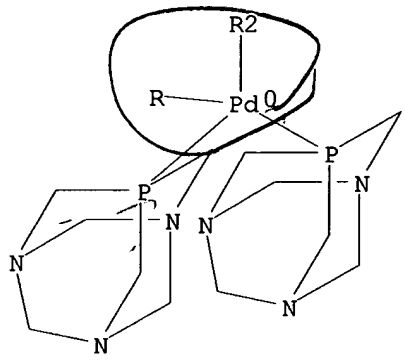
RN 106-99-0 HCAPLUS

CN 1,3-Butadiene (8CI, 9CI) (CA INDEX NAME)



IT **188747-92-4P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(prepn. and catalysis in oligomerization and telomerization of **butadiene**)
RN 188747-92-4 HCAPLUS
CN Palladium, tetrakis(1,3,5-triaza-7-phosphatricyclo[3.3.1.13,7]decane-.kappa.P7)-, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A



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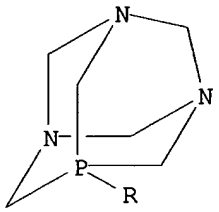
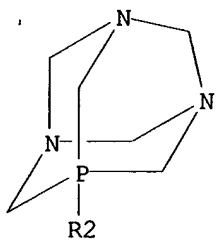


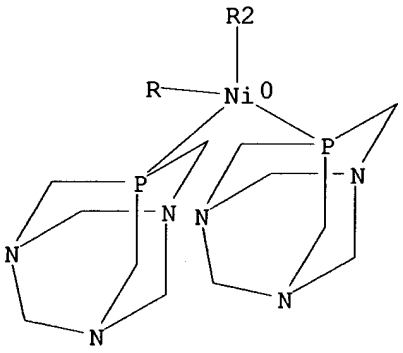


IT **188747-91-3P**

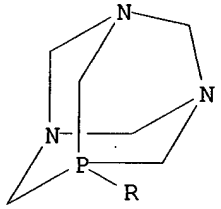
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(prepn. and lack of catalysis in oligomerization and telomerization of **butadiene**)

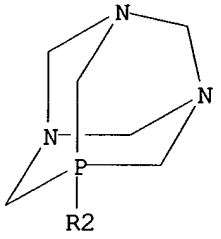
RN 188747-91-3 HCAPLUS
CN Nickel, tetrakis(1,3,5-triaza-7-phosphatricyclo[3.3.1.13,7]decane-.kappa.P7)-, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A





L15 ANSWER 12 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1996:202908 HCAPLUS
DOCUMENT NUMBER: 124:276831
TITLE: Synthesis of New Bidentate Phosphine Ligands Containing Saturated Phosphorus Heterocycles
AUTHOR(S): Field, Leslie D.; Thomas, Iain P.
CORPORATE SOURCE: Department Of Organic Chemistry, University of Sydney,

Sydney, 2006, Australia
SOURCE: Inorganic Chemistry (1996), 35(9), 2546-8
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis of two ethylene-bridged bidentate phosphines is described. 1,2-Bis(1-phospholano)ethane ((C4H8)PCH2CH2P(C4H8)) was synthesized by the stepwise addn. of 2,2-dioxo-1,3,2-dioxathiepane to H2PCH2CH2PH2. 1,2-Bis(1-phosphorinano)ethane ((C5H10)PCH2CH2P(C5H10)) was synthesized by the novel photochem. addn. of 1,4-pentadiene to H2PCH2CH2PH2. These bis(phosphines) form two-to-one complexes Fe(PP)2Cl2 when added to Fe(II) chloride.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 29

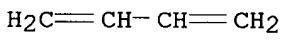
IT **106-99-0**, 1,3-**Butadiene**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(attempted reaction with lithium bis(phosphino)ethane)

IT **175551-12-9P 175551-13-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and sulfurization and complexation with iron)

IT **94033-45-1P 175551-14-1P** 175551-15-2P 175551-16-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

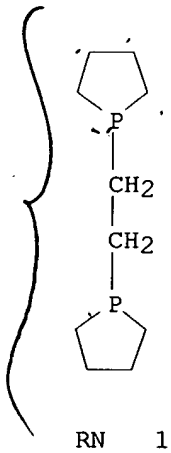
IT **106-99-0**, 1,3-**Butadiene**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(attempted reaction with lithium bis(phosphino)ethane)

RN 106-99-0 HCAPLUS
CN 1,3-Butadiene (8CI, 9CI) (CA INDEX NAME)



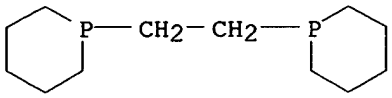
IT **175551-12-9P 175551-13-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and sulfurization and complexation with iron)

RN 175551-12-9 HCAPLUS
CN Phospholane, 1,1'-(1,2-ethanediyl)bis- (9CI) (CA INDEX NAME)

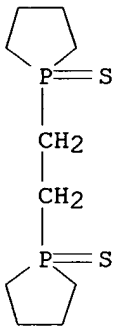


RN 175551-13-0 HCAPLUS

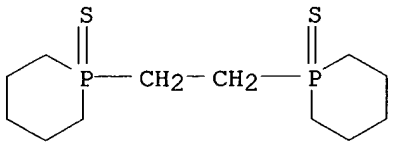
CN Phosphorinane, 1,1'-(1,2-ethanediyl)bis- (9CI) (CA INDEX NAME)



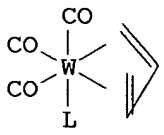
IT **94033-45-1P 175551-14-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 94033-45-1 HCAPLUS
CN Phospholane, 1,1'-(1,2-ethanediyl)bis-, 1,1'-disulfide (9CI) (CA INDEX NAME)



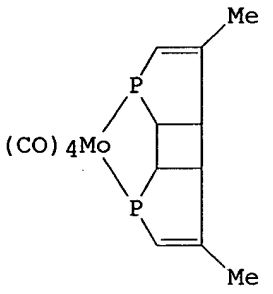
RN 175551-14-1 HCAPLUS
CN Phosphorinane, 1,1'-(1,2-ethanediyl)bis-, 1,1'-disulfide (9CI) (CA INDEX NAME)



L15 ANSWER 13 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1987:423441 HCAPLUS
DOCUMENT NUMBER: 107:23441
TITLE: Synthesis and stereochemical studies of tricarbonylphosphole-.eta.4-diene-metal(0) complexes of VIB Group elements
AUTHOR(S): Ozkar, Saim; Ozer, Zahide
CORPORATE SOURCE: ODTU Kimya Bolumu, Ankara, Turk.
SOURCE: Doga: Turk Kimya Dergisi (1986), 10(1), 53-68
CODEN: DKSEE7; ISSN: 1010-7614
DOCUMENT TYPE: Journal
LANGUAGE: Turkish
GI



III



IV

AB Q(CO)5L (I) and Q(CO)4L2 [II; Q = Cr, Mo, W; L = 1-phenyl-3,4-dimethylphosphole (pdp), 1-phenyl-3-methylphosphole (pmp) and 1-phenylphosphole] were synthesized photochem. from Q(CO)6 and the appropriate phosphole. The structure of these complexes were studied by IR and NMR spectroscopies. The octahedral II complexes existed in the cis form. I (Q = Cr, W; L = pdp) reacted with conjugated dienes under UV irradn. to give Q(CO)3L(diene). E.g., I (Q = W, L = pdp) reacted with 1,3-butadiene to give octahedral tricarbonyl(phosphole)(diene)tungsten III. The stereochem. of III was studied spectroscopically. II (Q = Mo, L = pmp) underwent photochem. intramol. dimerization to give molybdenum tetracarbonyl IV.

CC 29-11 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 78

ST molybdenum **carbonyl** phosphole photochem **diene**; chromium **carbonyl** phosphole photochem **diene**; tungsten **carbonyl** phosphole photochem **diene**

IT Molecular structure
(of **carbonyl**(phosphole)(**diene**)chromium, and -tungsten complexes)

IT **108589-24-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., multinuclear NMR and IR and photolysis of)

IT **74363-91-0P** 74363-92-1P **74391-02-9P** 94024-76-7P 108589-20-4P 108589-21-5P 108589-22-6P **108589-23-7P** **108589-25-9P** **108608-22-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., multinuclear NMR and IR of)

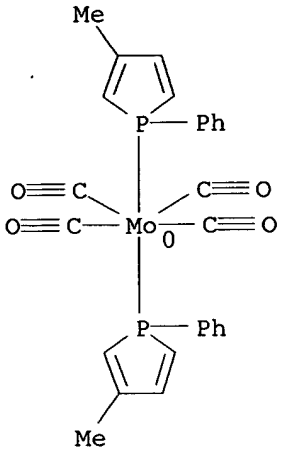
IT **108589-26-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn., photochem. substitution reaction, and NMR spectra of)

IT **106-99-0**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phospholetungsten and -chromium pentacarbonyl)

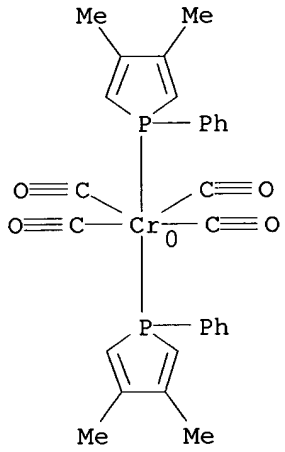
IT **108589-24-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., multinuclear NMR and IR and photolysis of)

RN 108589-24-8 HCAPLUS

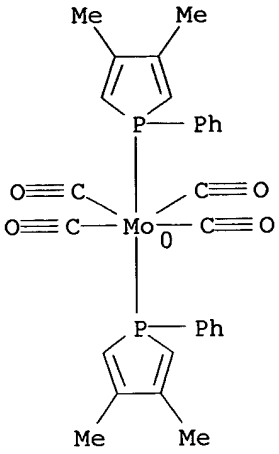
CN Molybdenum, tetracarbonylbis(3-methyl-1-phenyl-1H-phosphole)-, (OC-6-22)-(9CI) (CA INDEX NAME)



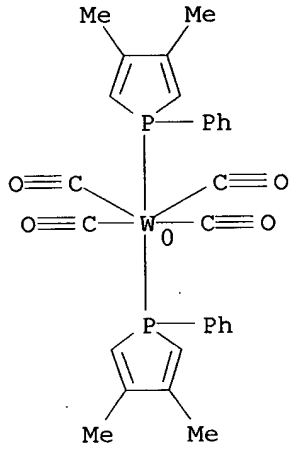
IT **74363-91-0P 74391-02-9P 108589-23-7P**
108589-25-9P 108608-22-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., multinuclear NMR and IR of)
RN 74363-91-0 HCAPLUS
CN Chromium, tetracarbonylbis(3,4-dimethyl-1-phenyl-1H-phosphole)-, (OC-6-22)- (9CI) (CA INDEX NAME)



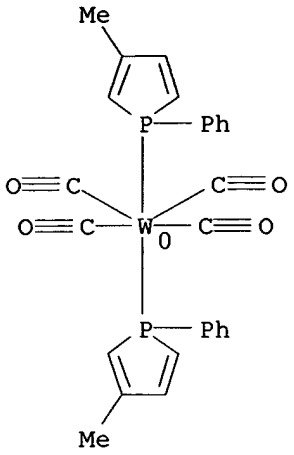
RN 74391-02-9 HCAPLUS
CN Molybdenum, tetracarbonylbis(3,4-dimethyl-1-phenyl-1H-phosphole)-, (OC-6-22)- (9CI) (CA INDEX NAME)



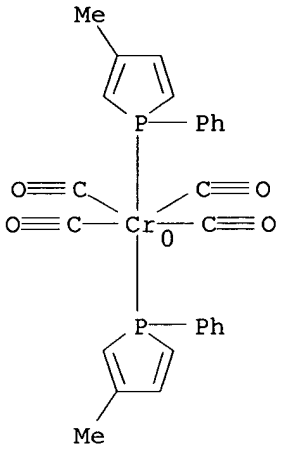
RN 108589-23-7 HCAPLUS
CN Tungsten, tetracarbonylbis(3,4-dimethyl-1-phenyl-1H-phosphole)-, (OC-6-22)- (9CI) (CA INDEX NAME)



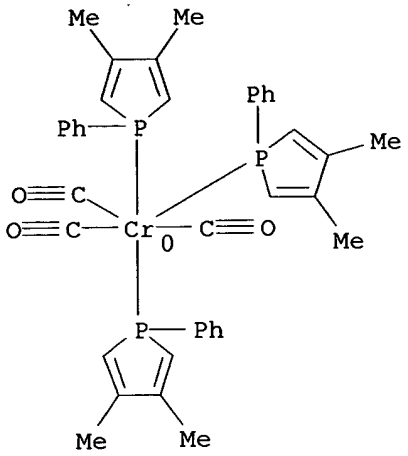
RN 108589-25-9 HCAPLUS
CN Tungsten, tetracarbonylbis(3-methyl-1-phenyl-1H-phosphole)-, (OC-6-22)- (9CI) (CA INDEX NAME)



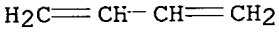
RN 108608-22-6 HCAPLUS
CN Chromium, tetracarbonylbis(3-methyl-1-phenyl-1H-phosphole)-, (OC-6-22)-(9CI) (CA INDEX NAME)



IT **108589-26-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn., photochem. substitution reaction, and NMR spectra of)
RN 108589-26-0 HCAPLUS
CN Chromium, tricarbonyltris(3,4-dimethyl-1-phenyl-1H-phosphole)-, (OC-6-22)-(9CI) (CA INDEX NAME)



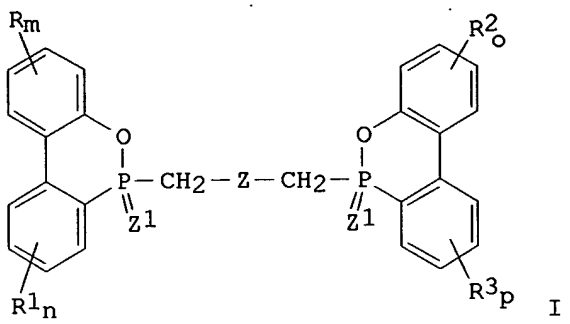
IT **106-99-0**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phospholetungsten and -chromium pentacarbonyl)
RN 106-99-0 HCAPLUS
CN 1,3-Butadiene (8CI, 9CI) (CA INDEX NAME)



L15 ANSWER 14 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1987:85749 HCAPLUS
DOCUMENT NUMBER: 106:85749
TITLE: Flame-retardant resin compositions
INVENTOR(S): Tsunetani, Masami
PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61162541	A2	19860723	JP 1985-2094	19850111
JP 06008371	B4	19940202		

PRIORITY APPLN. INFO.: JP 1985-2094 19850111
GI



I

AB Self-extinguishing resin compns. with good heat and mech. phys. properties contains 100 parts resin compns. contg. polyoxyphenylenes and styrene polymers, and 0.5-20 parts P-contg. compds. I (R, R1-3 = C1-8 alkyl, aryl, alkoxy; Z = C1-6 alkylene, arylene, NH, O, S; Z1 = O, S; m, n, o, p = 0-4), and, optionally, arom. phosphates. Thus, a blend of poly(2,6-dimethyl-1,4-phenylene ether) 50, rubber-modified polystyrene (contg. 14% polybutadiene) 50, and I (R = R1 = R2 = R3 = H; Z1 = O; Z = 4-methylphenol-2,6-diyl) 4.5 parts, injection molded at 280.degree., had combustion time 8 (av.) and 15 s (max.), heat distortion temp. 122.degree. (18.5 kg/cm2 load), and melt flow rate 4.3 g/10 min (250.degree., 10 kg/cm2 load), compared with complete combustion with dripping, 122.degree., and 2.2 g/10 min for test pieces without I.

IC ICM C08L025-04
ICS C08K005-53; C08L071-04

CC 37-6 (Plastics Manufacture and Processing)

IT Rubber, **butadiene**, uses and miscellaneous
RL: USES (Uses)
(polystyrene modified by, polyoxyphenylene blends, dibenzoxaphosphorin fireproofing agents for)

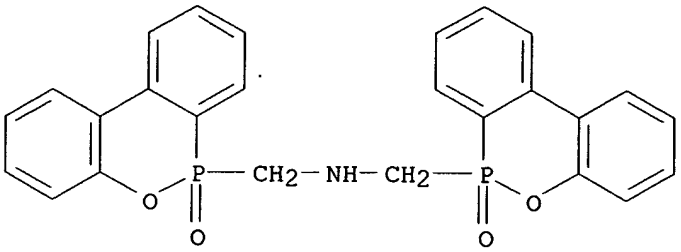
IT **106871-32-3** 106871-33-4
RL: USES (Uses)
(fireproofing agents, for polyoxyphenylene blends)

IT 9003-53-6, Polystyrene 9003-56-9, Acrylonitrile-**butadiene**-styrene copolymer
RL: PRP (Properties)
(polyoxyphenylene blends, dibenzoxaphosphorin fireproofing agents for)

IT **106871-32-3**
RL: USES (Uses)
(fireproofing agents, for polyoxyphenylene blends)

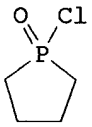
RN 106871-32-3 HCAPLUS

CN 6H-Dibenz[c,e][1,2]oxaphosphorin-6-methanamine, N-[(6-oxido-6H-dibenz[c,e][1,2]oxaphosphorin-6-yl)methyl]-, 6-oxide (9CI) (CA INDEX NAME)



L15 ANSWER 15 OF 22 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1985:96046 HCAPLUS
DOCUMENT NUMBER: 102:96046
TITLE: A new reagent for the mediation of amide bond formation in peptide synthesis
AUTHOR(S): Ramage, Robert; Ashton, Christopher P.; Hopton, David; Parrott, Maxwell J.
CORPORATE SOURCE: Inst. Sci. Technol., Univ. Manchester, Manchester, M60 1QD, UK
SOURCE: Tetrahedron Letters (1984), 25(42), 4825-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB The potential application of 1-oxo-1-chlorophospholane (I) as a novel reagent for the in situ activation of N.alpha.-protected amino acids for use in peptide bond forming reactions was examd. 31P NMR (3.4 MHz) was used to follow both the formation of the intermediate phospholanic-carboxylic mixed anhydride and the subsequent aminolysis reaction.

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 29

IT 7719-12-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with **butadiene**)

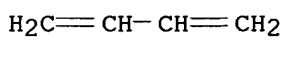
IT **106-99-0**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with phosphorus trichloride)

IT 7444-16-8P 10084-80-7P 39063-70-2P **46237-45-0P** 94989-51-2P 95015-12-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

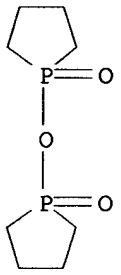
IT **106-99-0**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with phosphorus trichloride)

RN 106-99-0 HCAPLUS

CN 1,3-Butadiene (8CI, 9CI) (CA INDEX NAME)



IT **46237-45-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 46237-45-0 HCAPLUS
CN Phospholane, 1,1'-oxybis-, 1,1'-dioxide (9CI) (CA INDEX NAME)



L15 ANSWER 16 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1985:26127 HCAPLUS
DOCUMENT NUMBER: 102:26127
TITLE: Selective hydrogenation of carbon to carbon double bonds of a diene copolymer
INVENTOR(S): Rempel, Garry Llewellyn; Azizian, Hormoz
PATENT ASSIGNEE(S): Polysar Ltd., Can.
SOURCE: Fr. Demande, 16 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2540503	A1	19840810	FR 1983-19327	19831202
FR 2540503	B1	19861024		
CA 1203047	A1	19860408	CA 1982-417260	19821208
US 4503196	A	19850305	US 1983-541252	19831012

PRIORITY APPLN. INFO.: CA 1982-417260 19821208
AB Diene copolymers are hydrogenated, giving rubbers whose vulcanizates resist oxidn. at high temps. for long times, in org. solvents contg. the catalysts RhHLx (L = a ligand, x = 3 or 4). Thus, hydrogenation of nitrile rubber (34% nitrile, Krynack 34-50) as a 1.6% soln. in 10 mL PhCl contg. 25 mg (Ph3P)4RhH [18284-36-1] at 55.degree./0.09 MPa for 19 h gave 91% hydrogenation of double bonds.
IC C08F236-04; C08F008-04; B01J031-18; B01J031-24
CC 39-4 (Synthetic Elastomers and Natural Rubber)
Section cross-reference(s): 67
IT Rubber, **butadiene**-styrene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)

(triblock, hydrogenation of, catalysts for)
IT 18284-36-1 **52365-79-4** 75069-87-3
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for hydrogenation of diene copolymers)
IT **52365-79-4**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for hydrogenation of diene copolymers)
RN 52365-79-4 HCAPLUS
CN Rhodium, hydrotetrakis(5-phenyl-5H-benzo[b]phosphindole)-, (TB-5-12)-(9CI) (CA INDEX NAME)

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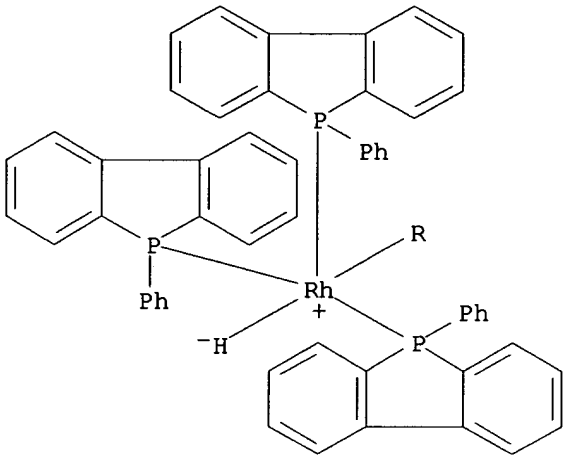

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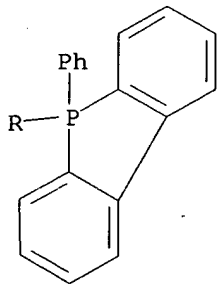


L15 ANSWER 17 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1983:5082 HCAPLUS
DOCUMENT NUMBER: 98:5082
TITLE: Light-resistant polyoxyphenylene blends
PATENT ASSIGNEE(S): Asahi-Dow Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent

LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 57105452	A2	19820630	JP 1980-179715	19801220

PRIORITY APPLN. INFO.: JP 1980-179715 19801220

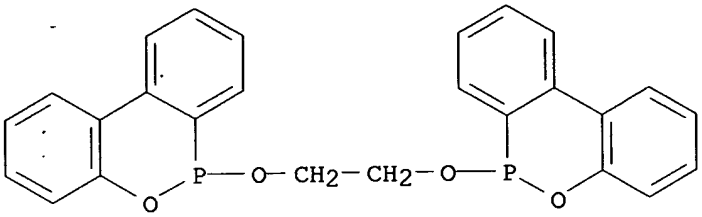
AB Impact-modified polyoxyphenylene compns. consisting of a polyoxyphenylene 20-60, an elastomeric polymer 0-30, and a styrene polymer 40-80% were incorporated, for improved light resistance with an aryl phosphonite 0.1-3, a UV absorber 0.1-3, and a sterically hindered phenol 0-2% (based on the final compn.), with the total stabilizer content being 0.2-8%. Thus, an extrusion-molded specimen from poly[oxy(2,6-dimethyl-1,4-phenylene)] [24938-67-8] 35, high-impact polystyrene [9003-53-6] 65, 10-(2,6-di-tert-butylphenoxy)-9,10-dihydro-9-oxa-10-phosphaphenanthrene (I) [9003-29-6] 10, and 2-(2-hydroxy-5-methylphenyl)benzotriazole [2440-22-4] 0.75 part had Izod impact strength 19 kg-cm/cm and impact strength retention (after 200 h in a weatherometer 63.degree. and relative humidity 50%) 83%, compared with 19 and 63, resp., for a control not contg. I.

IC C08L071-04; C08K005-50; C08K005-53; C08L025-04
ICI C08L071-04, C08L025-04, C08L021-00
CC 37-6 (Plastics Manufacture and Processing)
IT Rubber, **butadiene**, uses and miscellaneous
Rubber, **butadiene**-styrene, uses and miscellaneous
Rubber, nitrile, uses and miscellaneous
Rubber, synthetic
RL: USES (Uses)
(polyoxyphenylene blends, impact-resistant, light stabilizers for)

IT 79-74-3 85-28-9 85-60-9 88-24-4 88-58-4 90-68-6 94-01-9 96-66-2 96-69-5 118-55-8 118-82-1 119-47-1 128-37-0, uses and miscellaneous 131-54-4 131-55-5 131-56-6 131-57-7 976-56-7 991-84-4 1620-93-5 1709-70-2 1843-03-4 1843-05-6 2082-79-3 2162-63-2 2440-22-4 2658-23-3 2985-59-3 3135-18-0 3147-76-0 3147-77-1 3846-71-7 3864-99-1 3896-11-5 4192-61-4 5188-31-8 6683-19-8 13676-82-9 14894-91-8 15188-12-2 15618-85-6 17831-67-3 18824-08-3 22607-31-4 22617-00-1 23128-74-7 25973-55-1 27479-27-2 27676-62-6 30590-53-5 30596-65-7 30596-66-8 32509-66-3 33145-10-7 34137-09-2 35074-76-1 35074-77-2 36437-37-3 38080-24-9 38358-77-9 41484-35-9 57569-40-1 60699-47-0 70135-03-4 74734-21-7 **83937-11-5** 83937-12-6 83937-13-7 83937-14-8 83937-15-9 83937-16-0 83937-17-1 83937-18-2 83937-19-3 83937-20-6 83937-21-7 **83953-99-5** 83954-00-1
RL: USES (Uses)
(light stabilizers, for impact-modified polyoxyphenylene blends)

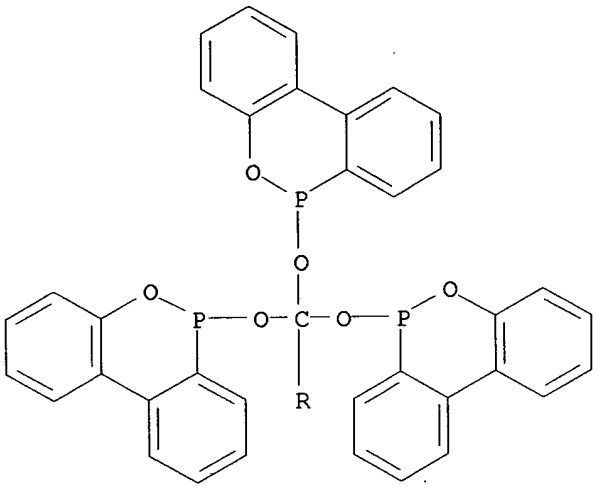
IT **83937-11-5 83953-99-5**
RL: USES (Uses)
(light stabilizers, for impact-modified polyoxyphenylene blends)

RN 83937-11-5 HCAPLUS
CN 6H-Dibenz[c,e][1,2]oxaphosphorin, 6,6'-[1,2-ethanediylbis(oxy)]bis- (9CI) (CA INDEX NAME)

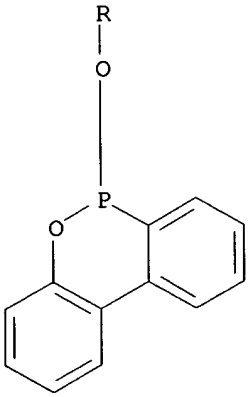


RN 83953-99-5 HCAPLUS
CN 6H-Dibenz[c,e][1,2]oxaphosphorin, 6,6',6'',6'''-[methanetetrayltetrakis(oxy)]tetrakis- (9CI) (CA INDEX NAME)

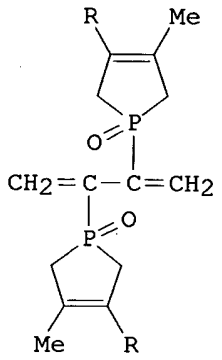
PAGE 1-A



PAGE 2-A

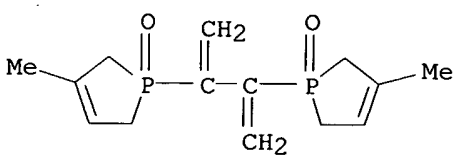


L15 ANSWER 18 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1981:481132 HCAPLUS
DOCUMENT NUMBER: 95:81132
TITLE: Synthesis and structure of diphospholenebutadienes
AUTHOR(S): Arbuzov, B. A.; Pudovik, A. N.; Vizel, A. O.; Shchukina, L. I.; Muslinkin, A. A.; Paramonova, V. I.; Kharitonov, V. V.; Krupnov, V. K.; Vakulenko, O. V.
CORPORATE SOURCE: Inst. Org. Fiz. Khim. im. Arbuzova, Kazan, USSR
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1981), (5), 1144-6
CODEN: IASKA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI

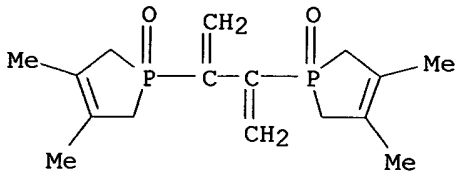


I

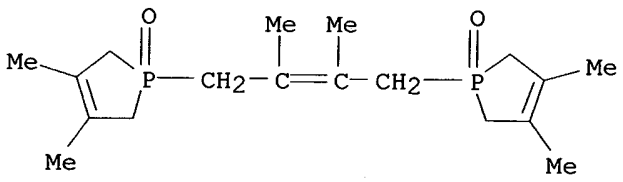
AB The title compds. I (R = H, Me) were obtained in 48.5-79.5% yields by treatment of HOCH2C.tplbond.CCH2OH with the corresponding 3-phospholene in THF contg. Et3N 24 h at 20.degree..
CC 29-7 (Organometallic and Organometalloidal Compounds)
ST diphospholenebutadiene; **butadiene** diphospholenyl
IT **78681-72-8P 78681-73-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **78681-72-8P 78681-73-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 78681-72-8 HCAPLUS
CN 1H-Phosphole, 1,1'-[1,2-bis(methylene)-1,2-ethanediyl]bis[2,5-dihydro-3-methyl-, 1,1'-dioxide (9CI) (CA INDEX NAME)



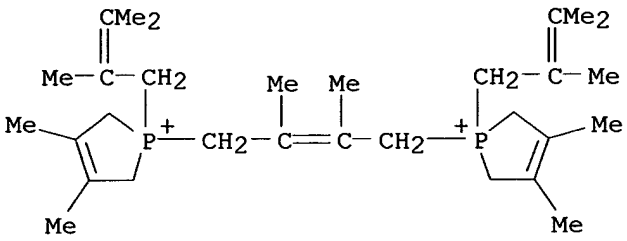
RN 78681-73-9 HCAPLUS
CN 1H-Phosphole, 1,1'-[1,2-bis(methylene)-1,2-ethanediyl]bis[2,5-dihydro-3,4-dimethyl-, 1,1'-dioxide (9CI) (CA INDEX NAME)



L15 ANSWER 19 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1976:44265 HCAPLUS
DOCUMENT NUMBER: 84:44265
TITLE: Reaction of 1-bromo-3,4-dimethylphosphol-3-ene with conjugated dienes
AUTHOR(S): Mathey, Francois; Thavard, Daniel
CORPORATE SOURCE: Inst. Natl. Rech. Chim. Appl., Vert-le-Petit, Fr.
SOURCE: Comptes Rendus des Seances de l'Academie des Sciences, Serie C: Sciences Chimiques (1975), 281(5-8), 243-5
CODEN: CHDCAQ; ISSN: 0567-6541
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB The reaction of 1-bromo-3,4-dimethyl-3-phospholene (I) with 2,3-dimethyl-1,3-butadiene followed by hydrolysis gave II (R = R1 = Me) (III), IV, and V (R = Br, Me2C:CMeCH2). The reaction I with butadiene and isoprene gave II (R = H, R1 = Me; R = R1 = H, Me resp.). III reacted with BzH and BzPh to give PhCR:CHCMe:CMeCH:CRPh (R = Ph, H, resp.).
CC 29-7 (Organometallic and Organometalloidal Compounds)
IT 31614-54-7P **57813-53-3P** 57813-54-4P **57813-55-5P** **57813-56-6P** **57813-57-7P** 57813-58-8P **57852-23-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 78-79-5, reactions **106-99-0**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(with bromophospholenes)
IT **57813-53-3P** **57813-55-5P** **57813-56-6P** **57813-57-7P** **57852-23-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 57813-53-3 HCAPLUS
CN 1H-Phosphole, 1,1'-(2,3-dimethyl-2-butene-1,4-diyl)bis[2,5-dihydro-3,4-dimethyl-, 1,1'-dioxide (9CI) (CA INDEX NAME)

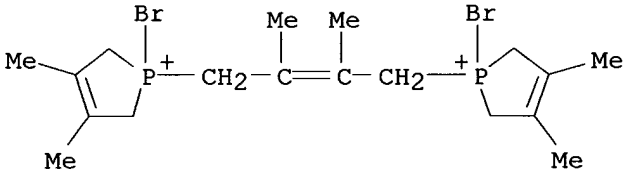


RN 57813-55-5 HCAPLUS
CN 1H-Phospholium, 1,1'-(2,3-dimethyl-2-butene-1,4-diyl)bis[1-(2,3-dimethyl-2-butenyl)-2,5-dihydro-3,4-dimethyl-, dibromide (9CI) (CA INDEX NAME)



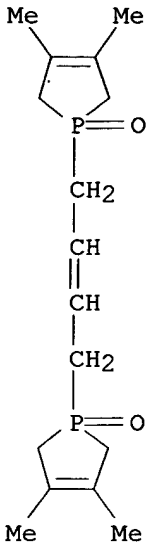
●2 Br^-

RN 57813-56-6 HCAPLUS
CN 1H-Phospholium, 1,1'-(2,3-dimethyl-2-butene-1,4-diyl)bis[1-bromo-2,5-dihydro-3,4-dimethyl-, dibromide (9CI) (CA INDEX NAME)

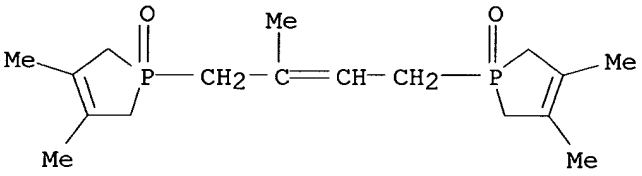


●2 Br^-

RN 57813-57-7 HCAPLUS
CN 1H-Phosphole, 1,1'-(2-butene-1,4-diyl)bis[2,5-dihydro-3,4-dimethyl-, 1,1'-dioxide (9CI) (CA INDEX NAME)



RN 57852-23-0 HCAPLUS
CN 1H-Phosphole, 1,1'-(2-methyl-2-butene-1,4-diyl)bis[2,5-dihydro-3,4-dimethyl-, 1,1'-dioxide (9CI) (CA INDEX NAME)



IT **106-99-0**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(with bromophospholenes)
RN 106-99-0 HCAPLUS
CN 1,3-Butadiene (8CI, 9CI) (CA INDEX NAME)

L15 ANSWER 20 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1972:449813 HCAPLUS
DOCUMENT NUMBER: 77:49813
TITLE: Polymerization catalysts derived from zero-valent state metal coordination complexes with group V-A compound
INVENTOR(S): Hawkins, John J.; Storrs, Charles D.; Zimmerman, Stanley D.
PATENT ASSIGNEE(S): Columbian Carbon Co.
SOURCE: U.S., 9 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent

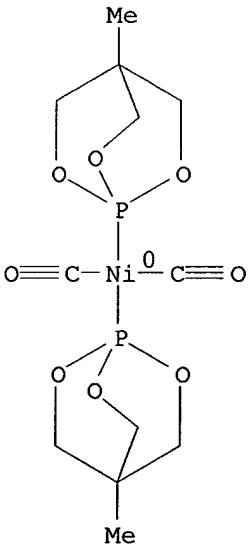
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3661882	A	19720509	US 1969-855753	19690905

PRIORITY APPLN. INFO.: US 1969-855753 19690905

AB Catalyst systems, comprised of coordination complexes such as tetrakis(triphenyl phosphite) nickel (I) [14221-00-2] or tris(triphenyl phosphite)nickel monocarbonyl (II) [14552-96-6] and an inorg. Lewis acid such as ZnCl2, were used with a solvent such as THF to polymerize olefinic compds. to crosslinkable linear polymers having a random distribution of trans and cis structures. Thus, a soln. of ZnCl2 in THF and a soln. of I in C6H6 were added to a polymn. reactor, butadiene added under pressure to the reactor, the mixt. polymd. at 120.deg. and 250 psig to give waxy polybutadiene [9003-17-2] having an unsatn. 1.74 moles/100 g and a trans-vinyl ratio of 13:1. 1,3-Butadiene-1,3-cyclooctadiene copolymer [35312-76-6] having a trans-vinyl-cis ratio 23:1:0 was prepd. similarly with the ZnCl2-II catalyst in C6H6.

IC C08D
NCL 260094300
CC 38-6 (Elastomers, Including Natural Rubber)
ST phosphite nickel polymn catalyst; Lewis acid polymn cocatalyst; **butadiene** polymn catalyst; structure polybutadiene; coordination complex polymn catalyst
IT 109-63-7 7637-07-2, uses and miscellaneous 13007-90-4
14262-94-3 15709-52-1 28042-59-3 37757-32-7 37837-62-0
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for polymn. of olefins)
IT **14262-94-3**
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for polymn. of olefins)
RN 14262-94-3 HCAPLUS
CN Nickel, dicarbonylbis(4-methyl-2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane-P1)-, (T-4)- (9CI) (CA INDEX NAME)



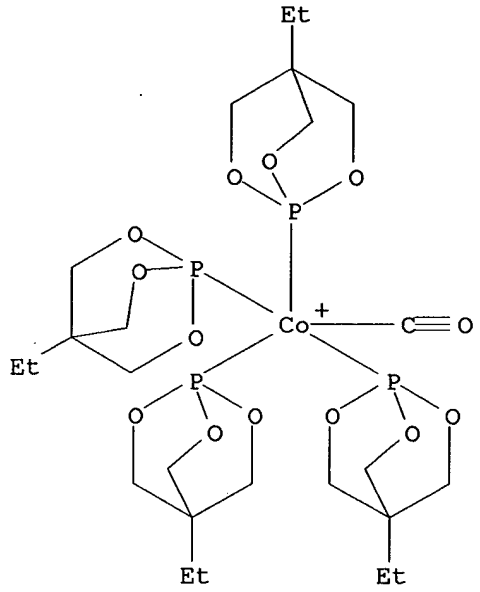
L15 ANSWER 21 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1970:85728 HCAPLUS
DOCUMENT NUMBER: 72:85728
TITLE: Carbonyl-bridged, phosphite-substituted cobalt carbonyl derivative
AUTHOR(S): Booth, Brian L.; Gardner, M.; Haszeldine, Robert N.
CORPORATE SOURCE: Univ. Manchester Inst. Sci. Technol., Manchester, UK
SOURCE: Journal of the Chemical Society [Section] D: Chemical Communications (1969), (23), 1388-9
CODEN: CCJDAO; ISSN: 0577-6171
DOCUMENT TYPE: Journal
LANGUAGE: English

AB HCo(CO)2L2[L = P(OCH2)3CEt] reacts with excess butadiene at room temp. for 7 days to give 60% [Co(CO)2L2]2, the ir spectra of which indicate that the complex contains CO bridges. [L2COCo(CO)2Co(CO)2L] (6% yield), 3% (.pi.-C4H7)Co(CO)L]2, 4% HCo(CO)L3, and 9% [Co(CO)2L3] [Co(CO)4] were alsoisolated. Co2(CO(8 and L were heated at 65-70.degree. for 30 hr in the absence of solvent to give 93% [Co(CO)L4] [Co(CO)4] which was identified by the prepn. of [Co(CO)L4]BPh4. The reaction of butadiene and HCo(CO)2[P(OPh)3]2 gave 47% of an unstable oil of the mol. formula [Co(CO)2[P(OPh)3]2]2 which was characterized by ir spectrum; 19% (.pi.-C4H7)Co(CO)[P(OPh)3]2was also isolated.

CC 78 (Inorganic Chemicals and Reactions)
ST carbonyls Co **butadiene** reactions; **butadiene** Co carbonyls reactions; cobalt carbonyls **butadiene** reactions; phosphito Co carbonyls reactions
IT 27636-55-1P **28134-06-7P 28301-14-6P 28301-15-7P 28451-46-9P 28709-56-0P 28709-57-1P 28713-43-1P** 29224-15-5P **29708-47-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **28134-06-7P 28301-14-6P 28301-15-7P 28451-46-9P 28709-56-0P 28709-57-1P 28713-43-1P 29708-47-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 28134-06-7 HCAPLUS
CN Cobalt(1+), carbonyltetrakis(phosphorous acid)-, tetraphenylborate(1-), cyclic tetraester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol, stereoisomer (8CI) (CA INDEX NAME)

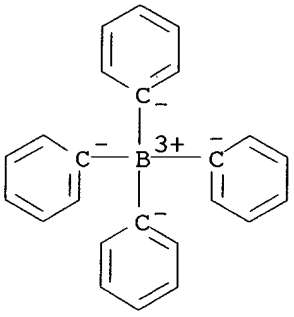
CM 1

CRN 47840-77-7
CMF C25 H44 Co O13 P4
CCI CCS

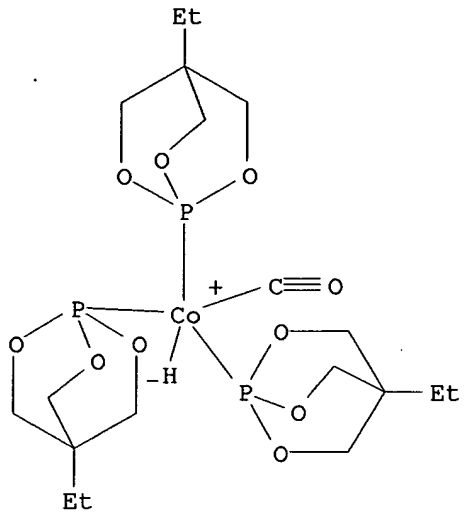


CM 2

CRN 4358-26-3
CMF C24 H20 B
CCI CCS



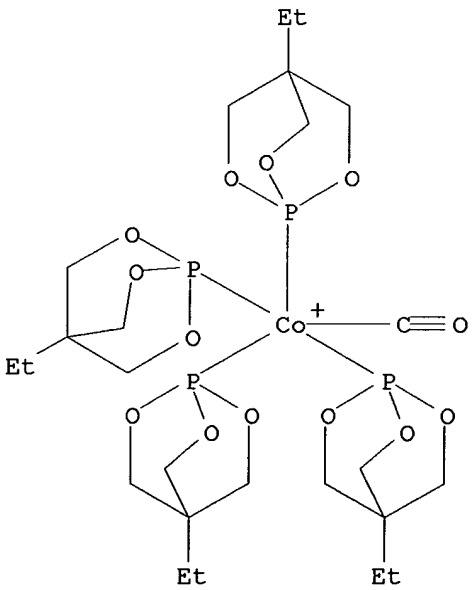
RN 28301-14-6 HCAPLUS
CN Cobalt, carbonylhydrotris(phosphorous acid)-, cyclic triester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol (8CI) (CA INDEX NAME)



RN 28301-15-7 HCAPLUS
CN Cobalt(1+), carbonyltetrakis(phosphorous acid)-, tetraphenylborate(1-), cyclic tetraester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol, stereoisomer (8CI) (CA INDEX NAME)

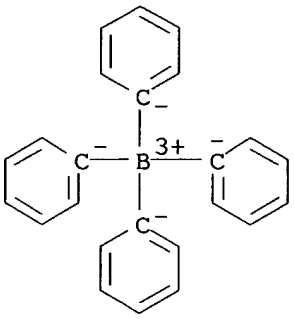
CM 1

CRN 47840-75-5
CMF C25 H44 Co O13 P4
CCI CCS



CM 2

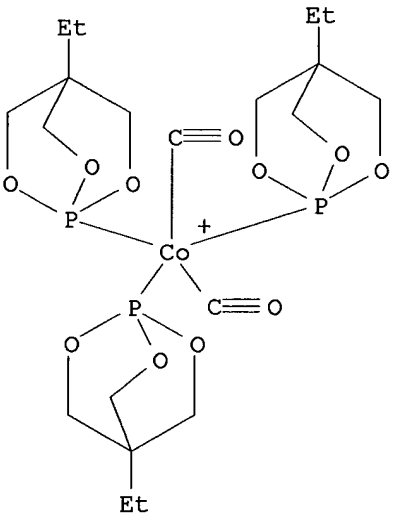
CRN 4358-26-3
CMF C24 H20 B
CCI CCS



RN 28451-46-9 HCAPLUS
CN Cobalt(1+), dicarbonyltris(4-ethyl-2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane-P1)-, tetraphenylborate(1-) (9CI) (CA INDEX NAME)

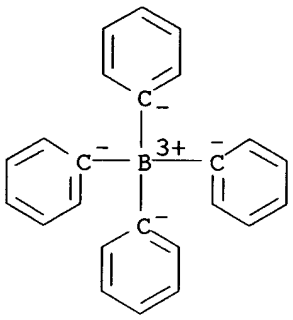
CM 1

CRN 47756-68-3
CMF C20 H33 Co O11 P3
CCI CCS



CM 2

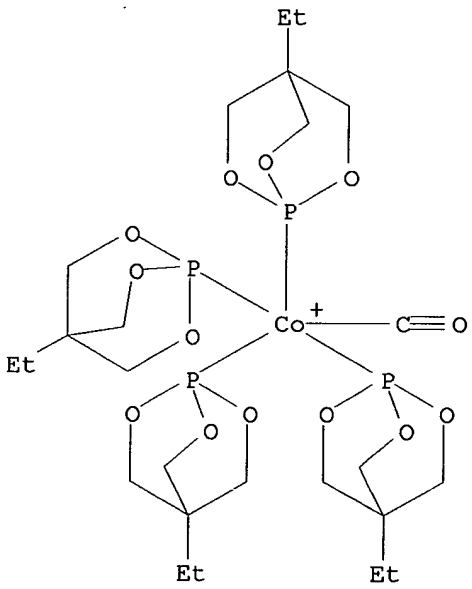
CRN 4358-26-3
CMF C24 H20 B
CCI CCS



RN 28709-56-0 HCAPLUS
CN Cobalt(1+), carbonyltetrakis(phosphorous acid)-, tetracarbonylcobaltate(1-), cyclic tetraester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol, stereoisomer (8CI) (CA INDEX NAME)

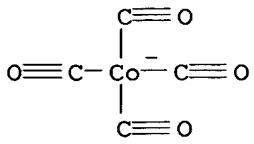
CM 1

CRN 47840-75-5
CMF C25 H44 Co O13 P4
CCI CCS



CM 2

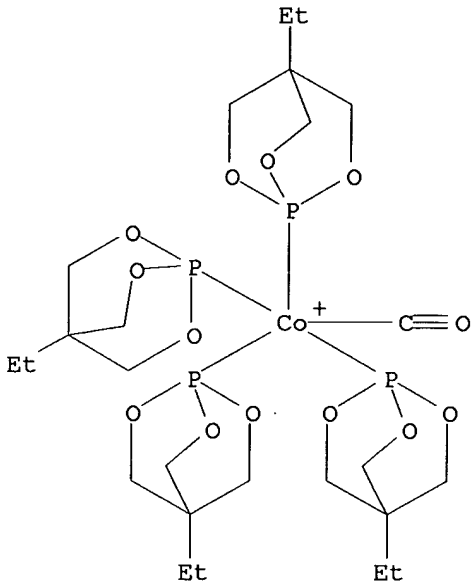
CRN 14971-27-8
CMF C4 Co O4
CCI CCS



RN 28709-57-1 HCAPLUS
CN Cobalt(1+), carbonyltetrakis(phosphorous acid)-, tetracarbonylcobaltate(1-), cyclic tetraester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol, stereoisomer (8CI) (CA INDEX NAME)

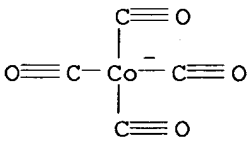
CM 1

CRN 47840-77-7
CMF C25 H44 Co O13 P4
CCI CCS



CM 2

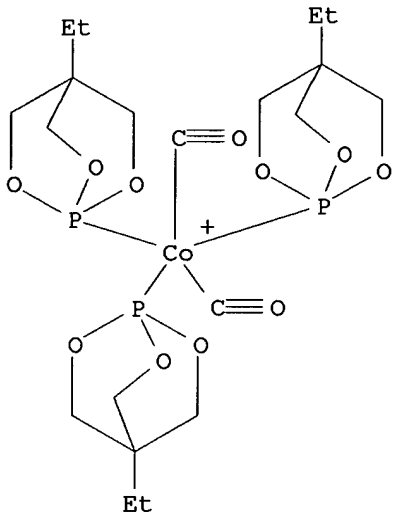
CRN 14971-27-8
CMF C4 Co O4
CCI CCS



RN 28713-43-1 HCAPLUS
CN Cobalt(1+), dicarbonyltris(phosphorous acid)-, tetracarbonylcobaltate(1-), cyclic triester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol (8CI) (CA INDEX NAME)

CM 1

CRN 47756-68-3
CMF C20 H33 Co O11 P3
CCI CCS



CM 2

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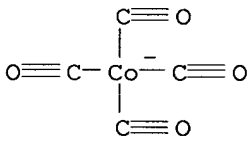
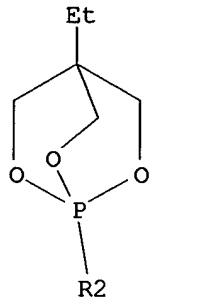
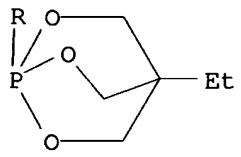


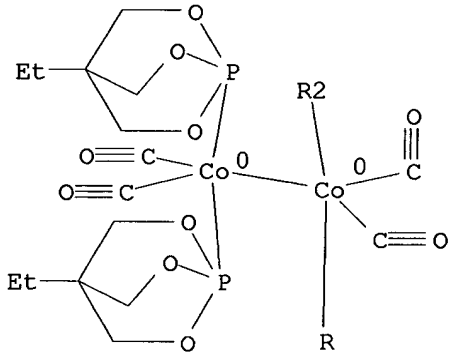
RN 29708-47-2 HCAPLUS
CN Cobalt, tetracarbonyltetrakis(phosphorous acid)di-, cyclic tetraester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol (8CI) (CA INDEX NAME)

PAGE 1-A





PAGE 2-A



L15 ANSWER 22 OF 22 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1965:454812 HCAPLUS
DOCUMENT NUMBER: 63:54812
ORIGINAL REFERENCE NO.: 63:9989c-f
TITLE: Cyclic dimers and trimers of linear conjugated diolefins
INVENTOR(S): Feldman, Julian; Saffer, Bernard A.; Thomas, Martin
PATENT ASSIGNEE(S): National Distillers and Chemical Corp.
SOURCE: 3 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 3194848		19650713	US	19621231

GI For diagram(s), see printed CA Issue.

AB The process consists in polymerizing a linear conjugated diolefin at 100-30.degree. in the presence of a catalyst A1.2-Ni-B2 in which A = 1-methyl-4phospha-3,5,8-trioxabicyclo(2.2.2)octane (I) and B = PhCH:CHCN (II), CH2>2: CHCH (III), CH2: CHCHO (IV) or carbonyl (V). A soln. of 36 g. (HOCH2)3CCH3 in 100 ml. anhyd. C5H5N dild. to 225 ml., was added simultaneously with 26.4 ml. PCl3 dild. to 225 ml. with tetrahydrofuran (under N) to 340 ml., the mixt. filtered, and the filtrate concd. in vacuo to a thick sirup from which I was removed by sublimation and crystd. from heptane. NiCO (8.6 g.) in a soln. of 13.4 g. II in 13 ml. Et2O was refluxed 4 hrs. to give Ni dicinnamonitrile (VI), a violet compd. which was washed with MeOH and Et2O, and dried. VI (0.69 g.) in a soln. of 0.76 g. I in 50 ml. Et2O was refluxed 8 hrs. to give 81% gray cryst. bis(I) Ni dicinnamonitrile. Ni diacrolein and mono-I Ni diacrolein were similarly obtained. To test the relative efficiencies of the various catalysts, polymerization reactions were carried out as follows. The stainless steel reactor (5/16 in. .times. 8 in.) (top covers connected to midget valves by means of glands and 1/16 in. stainless steel tubing, using Teflon gaskets to minimize leakage), purged with N was charged with 0.5 g. Ca2C (freshly ground under N), 0.3 ml. 1.07% soln. ptert-butylcatechol (inhibitor) in xylene, 1-5% catalyst and pressured to 200 psig. with O-free N. Approx. 6 ml. liquid butadiene (cooled in dry ice) was added (hypodermic syringe). The reactor was then purged (6 times) with N, the reaction mixt. heated to 120.degree. overnight and the products analyzed by vapor phase chromatography.

NCL 260666000

CC 39 (Organometallic and Organometalloidal Compounds)

IT 4904-61-4, 1,5,9-Cyclododecatriene
(manuf. of, from 1,3-**butadiene**, Ni complex catalysts in)

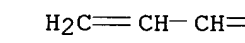
IT **106-99-0**, 1,3-**Butadiene**
(polymerization of, 4-methyl-2,6,7-trioxa-1-phosphabicyclo[2,2,2]octane Ni complexes as catalysts in)

IT 1449-91-8, 1,3-Propanediol, 2-(hydroxymethyl)-2-methyl-, cyclic phosphite 12148-53-7, Nickel, bis(cinnamonitrile)- 12266-60-3, Nickel, bis(acrolein)- **14655-09-5**, Nickel, bis(phosphorous acid)bis(cinnamonitrile)-, cyclic diester with 2-(hydroxymethyl)-2-methyl-1,3-propanediol
(prepn. of)

IT **106-99-0**, 1,3-**Butadiene**
(polymerization of, 4-methyl-2,6,7-trioxa-1-phosphabicyclo[2,2,2]octane Ni complexes as catalysts in)

RN 106-99-0 HCAPLUS

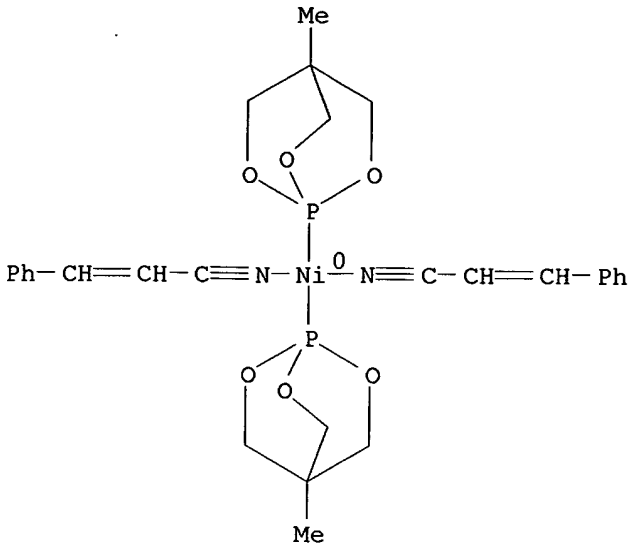
CN 1,3-Butadiene (8CI, 9CI) (CA INDEX NAME)



IT **14655-09-5**, Nickel, bis(phosphorous acid)bis(cinnamonitrile)-, cyclic diester with 2-(hydroxymethyl)-2-methyl-1,3-propanediol
(prepn. of)

RN 14655-09-5 HCAPLUS

CN Nickel, bis(4-methyl-2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane-P)bis(3-phenyl-2-propenenitrile)-, (T-4)- (9CI) (CA INDEX NAME)



D.CA IS NOT A RECOGNIZED COMMAND

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FILE 'WPIDS' ENTERED AT 08:41:00 ON 17 APR 2003
COPYRIGHT (C) 2003 THOMSON DERWENT

FILE LAST UPDATED:          16 APR 2003      <20030416/UP>
MOST RECENT DERWENT UPDATE:     200325        <200325/DW>
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>>> PATENT IMAGES AVAILABLE FOR PRINT AND DISPLAY <<<

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    PLEASE VISIT:
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    GUIDES, PLEASE VISIT:
    http://www.derwent.com/userguides/dwpi_guide.html <<<

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     (FILE 'WPIDS' ENTERED AT 08:34:48 ON 17 APR 2003)
                DEL HIS Y
L1          67747 S DIENE# OR BUTADIENE#
L2         273069 S CATALYS?
L3          12253 S L2 AND PHOSPHOR?
L4            647 S L1 AND L3
L5           3394 S  CARBONYLA?
L6             26 S L4 AND L5
L7         240059 S ALKANOL? OR ALC?
L8             20 S L6 AND L7
L9             96 S METHYL (2W)(PENTENOATE OR PENTENOIC)
L10           114 S  (DI METHYL OR METHYL)(2W)  ADIPATE OR  HEXANEDIOC ACID (2A)
L11           110 S L9 OR (DIMETHYL ) (2W) (PENTENOATE OR PENTENOIC)
L12           222 S L11 OR L10
L13             7 S L4 AND L12
L14             5 S L13 NOT L8

     FILE 'WPIDS' ENTERED AT 08:41:00 ON 17 APR 2003

=> d .wp l8 1-20;d .wp l14 1-5

L8   ANSWER 1 OF 20  WPIDS (C) 2003 THOMSON DERWENT
AN   2003-077585 [08]   WPIDS
DNC  C2003-020300
TI   Preparation of E-caprolactone, comprises carbonylating
     butadiene, hydroformylating, and reductively aminating to produce
     epsilon -caprolactam and epsilon -caprolactam precursors.
DC   A41 E13
IN   GUIT, R P M; HAASEN, N F; SIELCKEN, O; SMITS, H A; TINGE, J T; SIELCKEN, O
     E
PA   (STAM) DSM NV
CYC  101
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PI EP 1251122 A1 20021023 (200308)* EN 19p
R: AL AT BE CH CY DE DK ES FI FR GB GR IE IT LI LT LU LV MC MK NL PT RO SE SI TR
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W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT RO RU SD SE SG SI SK SL TJ TM TN TR TT TZ UA UG US UZ VN YU ZA ZM ZW

ADT EP 1251122 A1 EP 2001-201356 20010417; WO 2002083635 A1 WO 2002-NL250 20020417

PRAI EP 2001-201356 20010417

AB EP 1251122 A UPAB: 20030204

NOVELTY - Preparation of E-caprolactone starting from **butadiene**, carbon monoxide, hydrogen and ammonia comprises **carbonylating butadiene** to produce alkyl-pentenoate; hydroformylating the alkyl-4-, alkyl-3- and alkyl-2-pentenoate to produce alkyl-5-formylvalerate; and reductively aminating alkyl-5-formylvalerate to produce epsilon -caprolactam and epsilon -caprolactam precursors.

DETAILED DESCRIPTION - Preparation of E-caprolactone starting from **butadiene**, carbon monoxide, hydrogen and ammonia comprises:

(1) **carbonylating butadiene** in the presence of an **alkanol** and a **catalyst** comprising palladium, a multidentate phosphine ligand and an acidic co-**catalyst** to produce alkyl-4-, alkyl-3- and alkyl-2-pentenoate, (1') optionally isomerising the alkyl-3- and/or alkyl-2-pentenoate into alkyl-4-pentenoate,

(2) hydroformylating the alkyl-4-, alkyl-3- and alkyl-2-pentenoate in the presence of a **catalyst** comprising rhodium and an organic **phosphorous** containing ligand to produce alkyl-5-formylvalerate,

(3) reductively aminating alkyl-5-formylvalerate in the presence of a hydrogenation **catalyst** comprising ruthenium on a carrier **catalyst** to produce epsilon -caprolactam and epsilon -caprolactam precursors,

(4) optionally converting epsilon -caprolactam precursors at elevated temperature into epsilon -caprolactam.

INDEPENDENTS CLAIMS are included for E-caprolactam obtained by the process, and a composition containing:

(a) E-caprolactam; and

1-100 ppm 5-methyl-2-piperidinone and less than 10 ppm 4-ethyl-2-pyrrolidinone and/or 3-methyl-2-piperdinone.

USE - For the preparation of E-caprolactone.

ADVANTAGE - The process produces no ammonium sulfate by-product, uses cheaper and readily available starting materials, uses less energy, and has reduced emissions of nitrogen and/or sulfur oxides.

Dwg.0/0

TECH UPTX: 20030204

TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preferred Process: The multidentate phosphine ligand is a bidentate phosphine ligand selected from symmetric or asymmetric (3,3,1) or (4,2,1)isomers of 1,2-P,P'bis(1,5-dimethyl, 9-phosphabicyclononyl)ethane; 1,3-P,P'bis(1,5-dimethyl, 9-phosphabicyclononyl)propane; 1,2-P,P'bis (1,5-dimethyl 9-phosphabicyclononyl)propane. The organic **phosphorous** containing ligand is a multidentate phosphite ligand of formula (I): R1 and R2 = monovalent aromatic organic groups which are not connected to each other in any way other than via the **phosphorous** atom P;

R3 and R4 = substituents other than hydrogen, preferably carboalkoxyl, carboaryloxy group, or -CO2R;
R = 1-8C alkyl group;
A = n-valent group or atom, preferably a 2,2'-dihydroxyl-1,1'-binaphtalene bridging group of formula (II) or (III);
n = integer of at least 2; and
The phosphite forms a chelate-type complex with rhodium. The multidentate phosphite ligand is a bidentate phosphite ligand (n=2). The hydroformylation is performed in the presence of mono methyl adipate, and/or trio-tolylphosphine. The reductive amination is performed in the presence of a ruthenium on titanium oxide carrier hydrogenation **catalyst**, preferably in a water/corresponding **alkanol** mixture as solvent. The reductive amination step (3) is contacted with steam in the absence of a **catalyst** at 270 - 350 degreesC and a pressure below 1.5 MPa. The **alkanol** is separated from the mixture fed to the cyclisation step such that less than 1 wt.% of **alkanol** is present, and the separated **alkanol** is partly recycled to the **carbonylation** step (1). Caprolactam is isolated form the gaseous reaction mixture obtained in the cyclisation step by performing the following steps:
(A) the product stream is fed to a partial condensation unit and split in a top stream comprising steam and a liquid bottom stream comprising epsilon -caprolactam, water, lights and heavies;
(B) the bottom stream obtained in step A) is fed to a distillation column of which the top stream is mainly water and the bottom stream comprises epsilon -caprolactam, lights and heavies;
(C) the bottom stream obtained in step B) is fed to a vacuum distillation column of which the top stream is mainly lights and the bottom stream comprises epsilon -caprolactam and heavies;
(D) the bottom stream obtained in step C) is fed to a vacuum distillation column of which the top stream is the epsilon -caprolactam stream and the bottom stream is the heavies stream;
(E) the E-caprolactam stream obtained in step D) is fed into a crystallizer;
(F) the stream from the crystallizer is fed into a separater; and
(G) part of the mother liquor separated out in step F) is returned into the crystallizer.

L8 ANSWER 2 OF 20 WPIDS (C) 2003 THOMSON DERWENT
AN 2002-393928 [42] WPIDS
DNC C2002-110813
TI New ligands with two groups containing **phosphorus**, arsenic or antimony and other heteroatoms attached to a xanthene-type structure are used in group VIII metal complex **catalysts** for the hydroformylation of olefin to aldehyde and **alcohol**.
DC E19
IN AHLERS, W; BARTSCH, M; BAUMANN, R; HEWAT, A; PACIELLO, R; VOGT, D; WIEBELHAUS, D
PA (BADI) BASF AG
CYC 97
PI WO 2002022261 A2 20020321 (200242)* DE 39p
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ NL OA PT SD SE SL SZ TR TZ UG ZW
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ PH PL PT RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG US UZ VN YU ZA ZW
DE 10046026 A1 20020328 (200242)

AU 2002012250 A 20020326 (200251)
ADT WO 2002022261 A2 WO 2001-EP10735 20010917; DE 10046026 A1 DE 2000-10046026 20000918; AU 2002012250 A AU 2002-12250 20010917
FDT AU 2002012250 A Based on WO 200222261
PRAI DE 2000-10046026 20000918
AB WO 200222261 A UPAB: 20020704
NOVELTY - A method for the hydroformylation of olefinic compounds uses, as **catalysts**, complexes of group VIII metals with new ligands comprising compounds in which two groups containing **phosphorus**, arsenic or antimony and at least two other heteroatoms are attached to a xanthene-type structure at positions 4 and 5.

DETAILED DESCRIPTION - A method for the hydroformylation of olefinic compounds by reaction with carbon monoxide and hydrogen in presence of hydroformylation **catalysts** comprising complexes of group VIII metals new with ligands of formula (I).

A1, A2 = O, S, SiRaRb, NRc or CR5R6;

Ra, Rb, Rc, R5, R6 = H, alkyl, cycloalkyl, heterocycloalkyl, aryl or heteroaryl;

Y1, Y2 = **phosphorus**-, arsenic- or antimony-containing groups with at least two optionally substituted O, S and/or NRc atoms/groups directly attached to P, As or Sb (with Rc = H, alkyl, cycloalkyl or aryl);

R1-R4 = H, alkyl, cycloalkyl, heterocycloalkyl, aryl, heteroaryl, COORd, COO-M+, SO3Rd, SO3- M+, NE1E2, NE1E2E3+ X-, alkylene-NE1E2E3+ X-, ORd, SRd, (CHReCH2O)xRd, (CH2NE1)xRd, (CH2CH2NE1)xRd, halogen, trifluoromethyl, nitro, acyl or cyano, or R1 and/or R3 plus two adjacent carbon atoms in the benzene ring to which they are attached form a condensed ring system with 1, 2 or 3 other rings;

Rd, E1, E2, E3 = as for Rc;

Re = H, methyl or ethyl;

M = a cation;

X = an anion;

x = 1-120.

INDEPENDENT CLAIMS are also included for:

(a) compounds of formula (I);

(b) **catalysts** as described above.

USE - **Catalysts** containing (I) are used for hydroformylation, **carbonylation** and hydrogenation (claimed). The method is useful especially e.g. for the production of aldehydes and **alcohols** by hydroformylation of olefins.

ADVANTAGE - The **catalyst** enables the hydroformylation of alpha -olefins to give high yields of alpha -aldehydes or -**alcohols** and of internal linear olefins with high regioselectivity for terminal aldehydes. The **catalyst** has high activity and high stability under reaction conditions (i.e. long service life).

Dwg.0/0

TECH UPTX: 20020704

TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preferred Compounds: compounds of formula (I.1), (I.2), (I.3), (I.4), (I.5) and (I.6).

Ar = phenyl substituted with two groups as listed for R1-R4;

A = 1,2-phenylene, substituted with two groups as listed for R1-R4.

Preparation (disclosed): (I) may be obtained e.g. from the corresponding dihalo or similarly functionalized compounds (Y1, Y2 = halogen etc.) by lithiation followed by reaction with suitable organophosphorus halides.

Preferred **Catalysts**: Complexes of (I) with cobalt, ruthenium, iridium, rhodium, palladium or platinum, possibly with other ligand(s) selected from halides, amines, carboxylates, acetylacetonate, aryl- or alkyl-sulfonates, hydride, carbon monoxide, olefins, **dienes**,

cyclo-olefins, nitrogen heterocycles, aromatics and heteroaromatics, ethers, PF3, phospholes, phosphabenzenes and mono-, bi- or multi-dentate phosphine, phosphinite, phosphonite, **phosphoramidite** or phosphite ligands.
Preferred Olefins: Internal linear olefins and mixtures containing at least one of these.

L8 ANSWER 3 OF 20 WPIDS (C) 2003 THOMSON DERWENT
AN 2002-293303 [34] WPIDS
DNC C2002-086383
TI Preparation of dihydro- or carba-hydro addition products of olefins, involves using group VIII metal complex with bis-phospholyl-metallocene ligand as **catalyst** giving good selectivity.
DC A60 E11 E19 H04 J04
IN AHLERS, W; LE FLOCH, P; MACKEWITZ, T; MATHEY, F; PACIELLO, R; SAVA, X
PA (BADI) BASF AG
CYC 23
PI DE 10033982 A1 20020124 (200234)* 18p
WO 2002005955 A1 20020124 (200234) DE
RW: AT BE CH CY DE DK ES FI FR GB GR IE IT LU MC NL PT SE TR
W: CN JP US
EP 1299190 A1 20030409 (200325) DE
R: AT BE CH CY DE DK ES FI FR GB GR IE IT LI LU MC NL PT SE TR
ADT DE 10033982 A1 DE 2000-10033982 20000713; WO 2002005955 A1 WO 2001-EP8162 20010713; EP 1299190 A1 EP 2001-955349 20010713, WO 2001-EP8162 20010713
FDT EP 1299190 A1 Based on WO 200205955
PRAI DE 2000-10033982 20000713
AB DE 10033982 A UPAB: 20020528
NOVELTY - The preparation of 1,2-dihydro- and 1-hydro-2-carbo-addition products of the C=C double bonds of mono- or poly-ethylenically unsaturated compounds (A) involves addition reaction in presence of a **catalyst** (I) consisting of at least one complex of a group VIII transition metal having at least one bis-phospholyl-metallocene (II) (or its cation) as ligand.
DETAILED DESCRIPTION - INDEPENDENT CLAIMS is included for:
(1) **catalysts** (I); and
(2) bis-phospholyl-metallocenes of formula (II) and their cations.
M = group III or IV non-transition metal or group V-VIII transition metal;
n = 0-6;
L = ligand;
R5, R8, R'5, R'8 = heteroaryl substituted by 0-3 groups Q; or aryl substituted by 1-3 groups Q;
Q = alkyl, cycloalkyl, aryl, alkoxy, cycloalkoxy, aryloxy, acyl, halo, CF3, NO2, CN, COOH, alkoxycarbonyl or NA5A6;
R6, R7, R'6, R'7 = H, alkyl, heterocycloalkyl, aryl, heteroaryl, COORa, COOT, SO3Ra, SO3T, NA1A2, alkylene-NA1A2, NA1A2A3+.X-, alkylene-NA1A2A3+.X-, ORa, SRa, (CHRbCH2O)xRa, (CH2N(A1))xRa or (CH2CH2N(A1))xRa;
Ra, A1 - A3, A5, A6 = H, alkyl, cycloalkyl or aryl;
Rb = H, methyl or ethyl;
T = cation;
X = anion;
x = 1-120.
USE - The use of the **catalysts** (I) is claimed for hydroformylation, hydrocyanation, **carbonylation**, hydrogenation, olefin oligomerization/polymerization or metathesis. The claims also cover methods for the hydroformylation, hydrocyanation or **carbonylation**

of (A), involving reacting (A) with carbon monoxide, hydrogen cyanide or carbon monoxide/nucleophilic compound respectively in presence of (I). (I) are especially useful for catalyzing the hydroformylation of alpha -olefins to give products having as a high content of alpha -aldehydes or alpha -**alcohols** as possible.

ADVANTAGE - (I) have good catalytic activity and provide high selectivity, especially in the hydroformylation of alpha -olefins.

Dwg.0/0

TECH UPTX: 20020528

TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preferred **Catalysts**: (II) has at least two eta5-coordinated mono- or polyphospholene ligands, preferably of formula (IV).

E1-E4 = N, P, SiR or CR;

R = H, alkyl, cycloalkyl, heterocycloalkyl, aryl, heteroaryl, COORa, COOT, SO3Ra, SO3T, NA1A2, alkylene-NA1A2, NA1A2A3+.X-, alkylene-NA1A2A3+.X-, ORa, SRa, (CHRbCH2O)xRa, (CH2N(A1))xRa or (CH2CH2N(A1))xRa; or bridging group covalently linking two same or different ligands (IV) (coordinated with the same or different metals);

or two adjacent R groups together = fused ring.

Nine classes of preferred metallocenes (II) (including their cations) are specified in the claims, e.g. those of formula (III) or analogs of (III) in which:

(i) CR4 or CR3 is replaced by P,

(ii) R1 + R2 form a fused benzene or

(iii) R1 + R2 and R3 + R4 both form fused benzene rings.

R1 - R4, R'1 - R'4 = H, alkyl, cycloalkyl, heterocycloalkyl, aryl, heteroaryl, COORa, COOT, SO3Ra, SO3T, NA1A2, alkylene-NA1A2, NA1A2A3+.X-, alkylene-NA1A2A3+.X-, ORa, SRa, (CHRbCH2O)xRa, (CH2N(A1))xRa or (CH2CH2N(A1))xRa.

Catalysts (I) optionally comprises further ligands selected from halides, amines, carboxylates, acetylacetonate, aryl or alkylsulfonates, hydride, carbon monoxide, olefins, **dienes**, cycloolefins, nitriles, N-containing heterocycles, aromatics or heteroaromatics, ethers, **phosphorus** trifluoride, phosphabenzenes, and mono-, do- or polydentate phosphine, phosphinite, phosphonite, **phosphoramidite** and phosphite ligands.

Preparation: (II) are prepared by reacting the phospholyl ligand(s) with metal powder, compound or complex in a solvent.

L8 ANSWER 4 OF 20 WPIDS (C) 2003 THOMSON DERWENT

AN 2002-292471 [33] WPIDS

DNC C2002-085959

TI **Carbonylation** process involves reacting a conjugated **diene** with carbon monoxide and hydroxyl-containing compound in the presence of a **catalyst** comprising palladium, diphosphine ligand and anion source.

DC E19

IN DRENT, E; JAGER, W W; SIELCKEN, O E; TOTH, I

PA (STAM) DSM NV

CYC 96

PI WO 2002026690 A1 20020404 (200233)* EN 28p

RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ NL OA PT SD SE SL SZ TR TZ UG ZW

W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ PL PT RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG US UZ VN YU ZA ZW

AU 2002011067 A 20020408 (200252)

ADT WO 2002026690 A1 WO 2001-NL709 20010926; AU 2002011067 A AU 2002-11067 20010926
FDT AU 2002011067 A Based on WO 200226690
PRAI EP 2000-203356 20000927; EP 2000-203355 20000927
AB WO 200226690 A UPAB: 20020524
NOVELTY - A conjugated **diene** is **carbonylated** by reaction with carbon monoxide and a hydroxyl-containing compound in the presence of a **catalyst** comprising palladium, a ligand containing two **phosphorus**-containing rings, and an anion source.

DETAILED DESCRIPTION - **Carbonylation** of a conjugated **diene** involves reacting the conjugated **diene** with carbon monoxide and a hydroxyl group-containing compound in the presence of a **catalyst** comprising:

(a) a palladium cation source;
(b) a diphosphine ligand of formula (I); and
(c) a source of anions.

X1-R-X2 (I)

X1, X2 = a **phosphorus**-containing cyclic group of at least 5 ring atoms; and

R = an aliphatic bridging group containing 2-4 bridging atoms substituted with at least one substituent, or 1,2-phenylene.

An INDEPENDENT CLAIM is included for a **catalyst** system comprising:

(a) a palladium cation source;
(b) a diphosphine ligand of formula (I) in which R is any organic bridging group;
(c) a source of anions derived from a tertiary carboxylic acid of formula (II); and
(d) a substoichiometric amount of halide anions.

A proviso is given that the **catalyst** system contains less than 0.5 mole of an anion, other than halide anions, that is the conjugated base of an acid having a pKa less than 3, per mole palladium cations.

R4, R5, R6 = alkyl or aryl, preferably at least one is methyl or ethyl.

USE - The **carbonylation** process is useful for the preparation of alkyl pentenoates and adipates.

ADVANTAGE - The **catalyst** system has good activity, remains stable over a prolonged time period and can be reused several times without substantial loss of activity.

Dwg.0/0

TECH UPTX: 20020524
TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preferred Materials: The conjugated **diene** is 1,3-**butadiene**. The hydroxyl group-containing compound is a 1-20C **alkanol** or 2-20C alkanediol.
Preferred **Catalyst**: The molar ratio of halide anions to palladium cations is 0.001:1 - 1.5:1. The halide ions are preferably iodide ions, provided by hydrogen iodide.

L8 ANSWER 5 OF 20 WPIDS (C) 2003 THOMSON DERWENT
AN 2002-055128 [07] WPIDS
CR 2001-590030 [66]
DNC C2002-015667
TI Preparation of 5-cyanovaleric acid or its ester by using **catalyst** system including metal of Group VIII or its compound, bidentate phosphine, arsine, and/or stibine ligand, and acid.
DC A41 E13 E16
IN DRENT, E; JAGER, W W

PA (SHEL) SHELL INT RES MIJ BV; (DREN-I) DRENT E; (JAGE-I) JAGER W W
CYC 95
PI WO 2001072697 A2 20011004 (200207)* EN 23p
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ NL OA PT SD SE SL SZ TR TZ UG ZW
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CR CU CZ DE DK DM DZ EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ PL PT RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG UZ VN YU ZA ZW
AU 2001050380 A 20011008 (200208)
US 2002045748 A1 20020418 (200228)
EP 1263713 A2 20021211 (200301) EN
R: AL AT BE CH CY DE DK ES FI FR GB GR IE IT LI LT LU LV MC MK NL PT RO SE SI TR
BR 2001009239 A 20021224 (200309)
ADT WO 2001072697 A2 WO 2001-EP2903 20010314; AU 2001050380 A AU 2001-50380 20010314; US 2002045748 A1 US 2001-804891 20010313; EP 1263713 A2 EP 2001-923664 20010314, WO 2001-EP2903 20010314; BR 2001009239 A BR 2001-9239 20010314, WO 2001-EP2903 20010314
FDT AU 2001050380 A Based on WO 200172697; EP 1263713 A2 Based on WO 200172697; BR 2001009239 A Based on WO 200172697
PRAI EP 2000-200927 20000314; EP 2000-200926 20000314
AB WO 200172697 A UPAB: 20030206
NOVELTY - A 5-cyanovaleric acid or its ester is prepared by using a **catalyst** system comprising a metal of Group VIII or its compound in the periodic table of elements; a bidentate phosphine, arsine, and/or stibine ligand; and an acid having a pKa less than 3 at 18 deg. C in an aqueous solution.

DETAILED DESCRIPTION - Preparation of a 5-cyanovaleric acid or its ester involves reacting pentene-nitrile with carbon monoxide and water or an **alcohol** in the presence of a **catalyst** system. The **catalyst** system comprises a metal of Group VIII or its compound in the periodic table of elements; a bidentate phosphine, arsine, and/or stibine ligand; and an acid having a pKa less than 3 at 18 deg. C in an aqueous solution. The bidantate ligand is of formula R1R2-M1-R-M2-R3R4.

M1, M2 = P, As, or Sb;

R = divalent organic bridging group comprising a chain of 3-5 atoms directly connecting the 2 **phosphorus** atoms (the chain comprises carbon and optionally nitrogen, oxygen or sulfur or a silano or dialkylsilicon comprising 1-4C;

R1-R4 = optionally substituted tert. alkyl.

An INDEPENDENT CLAIM is also included for a process of preparing epsilon -caprolactam from pentenenitrile comprising **carbonylation** of pentenenitrile to the inventive 5-cyanovaleric acid or ester, reduction of 5-cyanovaleric acid or ester to 6-aminocaproic acid or ester, and cyclization of the 6-aminocaproic acid or ester to epsilon -caprolactam.

USE - For preparing 5-cyanovaleric acid or its ester useful in the preparation of epsilon -caprolactam and useful as intermediate to prepare adipic acid or its ester.

ADVANTAGE - The invention can be performed at a low temperature and has an overall selectivity of 90%, based on **butadiene**, to epsilon -caprolactam. It can be obtained in high yield under process conditions, which are mild with respect to operating pressure and/or temperature.

Dwg.0/0

TECH UPTX: 20020130
TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preferred Component: The bidantate ligand is a biphosphine ligand, preferably 1,3-bis(di-tert.butylphosphino)-

propane or 1,2-bis(di-tert.butylphosphinomethyl)benzene.
Preferred Ratio: The molar ratio of the ligand and metal is 1:1-5:1. The molar ratio of the acid and metal is 1:1-5:1.
Preferred Process: The temperature is 80-125 degreesC.
A mixture of branched and linear **carbonylation** products as obtained in the **carbonylation** is used in the reduction and/or cyclization.

TECHNOLOGY FOCUS - INORGANIC CHEMISTRY - Preferred Component: The metal is palladium.

L8 ANSWER 6 OF 20 WPIDS (C) 2003 THOMSON DERWENT
AN 2002-025717 [03] WPIDS
DNC C2002-007060
TI Separation of products from reaction product fluid comprising metal-organophosphorous ligand complex **catalyst** involves subjecting reaction product fluid to fractional countercurrent extraction.
DC A17 E11 J01 J04
IN ARGYROPOULOS, J N; BRIGGS, J R; BRYANT, D R; KANEL, J S; LEE, M M; MAHER, J M; PHILLIPS, A G; ROESCH, B M
PA (UNIC) UNION CARBIDE CHEM & PLASTICS TECHNOLOGY
CYC 91
PI WO 2001068251 A2 20010920 (200203)* EN 64p
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ NL OA PT SD SE SL SZ TR TZ UG ZW
W: AE AL AM AT AU AZ BA BB BG BR BY CA CH CN CR CU CZ DE DK DM EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX NO NZ PL PT RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG UZ VN YU ZA ZW
US 6303829 B1 20011016 (200203)
AU 2001045722 A 20010924 (200208)
ADT WO 2001068251 A2 WO 2001-US8180 20010314; US 6303829 B1 US 2000-526434 20000315; AU 2001045722 A AU 2001-45722 20010314
FDT AU 2001045722 A Based on WO 200168251
PRAI US 2000-526434 20000315
AB WO 200168251 A UPAB: 20020114
NOVELTY - Products are separated from a reaction product fluid comprising metal-organophosphorous ligand complex **catalyst** by subjecting the reaction product fluid to fractional countercurrent extraction with at least two immiscible extraction solvents comprising both polar and nonpolar extraction solvents to obtain a nonpolar phase and a polar phase; and recovering the polar phase from the nonpolar phase.
DETAILED DESCRIPTION - Separation of products from a reaction product fluid comprising metal-organophosphorous ligand complex **catalyst**, optionally free organophosphorous ligand, reaction product(s), non-polar reaction solvent(s), and polar reaction solvent(s) involves (a) subjecting the reaction product fluid to fractional countercurrent extraction with at least two immiscible extraction solvents comprising both polar and nonpolar extraction solvents to obtain a nonpolar phase and a polar phase; and (b) recovering the polar phase from the nonpolar phase. The nonpolar phase includes the **catalyst**, the ligand, nonpolar reaction solvent(s), and nonpolar extraction solvent. The polar phase includes the reaction product, polar reaction solvent(s), and polar extraction solvent(s). The organophosphorous ligand has a partition coefficient (Kp1) between the nonpolar phase and the polar phase expressed as the quotient of the concentration of organophosphorous ligand in the nonpolar and polar phase after extraction. Kp1 is greater than 5. The reaction product(s) has a partition coefficient (Kp2) between the nonpolar and polar phase

expressed as the quotient of the products in the nonpolar and polar phase after extraction. Kp2 is less than 2.

USE - The method is for separating desired product, along with organophosphorous ligand degradation product(s) and reaction byproducts from a reaction product fluid. It is used in preparing **alcohols**, amines, amides, ethers, epoxides, esters, ketones, aldehydes, and nitriles.

ADVANTAGE - The invention makes it possible to separate desired product, and other reaction byproducts, from the reaction product fluid without the need to use vaporization separation and the harsh conditions associated with such processes. It provides highly desirable separation method that prevents and lessens the buildup of organophosphorous ligand degradation products and reaction byproducts in the reaction product fluid. Use of the fractional countercurrent extraction instead of conventional extraction, results to lower **catalysts** costs resulting from more efficient recovery of **catalysts** from product, reduction in reactor volume and costs resulting from more efficient recovery of product from **catalyst**, improved operability in the extractor, lower investment costs based on less equipment, and reduced investment and operating costs resulting from improved partition coefficients of solute(s).

Dwg.0/0

TECH UPTX: 20020114

TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preferred Process: The method includes hydroformylation, hydroacylation (intramolecular and intermolecular), hydrocyanation, hydroamidation, hydroesterification, aminolysis, **alcoholysis**, hydrocarbonylation, reductive hydroformylation, hydrogenation, oligomerization, hydroxycarbonylation, **carbonylation**, isomerization, or transfer hydrogenation. The products are derivatized by hydrogenation, esterification, etherification, amination, alkylation, dehydrogenation, reduction, acylation, condensation, carboxylation, **carbonylation**, oxidation, cyclization, reductive amination, silylation, hydrolysis, and/or polymerization.

Preferred Value: Kp1 is greater than 7.5 and Kp2 is greater than 1.5. The selectivity of the nonpolar phase for the organophosphorous ligand with respect to the product(s) is expressed by the partition coefficient ratio Ef1 which is Kp1/Kp2. The selectivity of the nonpolar phase for the organophosphorous ligand with respect to organophosphorous ligand degradation product(s) is expressed by partition coefficient ratio Ef2 which is the quotient of Kp1 and Kp3 (partition coefficient of organophosphorous ligand degradation product(s)). Kp3 is the ratio of the concentration of organophosphorous ligand degradation products in the nonpolar to the polar phase after extraction. Ef1 is greater than 2.5 (preferably greater than 3.0), Ef2 is greater than 3, and Ef3 is greater than 2.5 (preferably greater than 3). Preferred **Catalyst**: The metal-organophosphorous ligand complex **catalyst** comprises rhodium complexed with a triorganophosphine ligand of formula (I), a mono-, di-, or tri-organophosphite of formula (II), (III) or (IV) respectively, and an organopolyphosphite containing two or more tertiary (trivalent) **phosphorus** atoms of formula (V).

R1 = optionally substituted at least 1-24C monovalent hydrocarbon radical;

R3 = optionally substituted at least 4-40C trivalent hydrocarbon radical;

R4 = optionally substituted at least 4-40C divalent hydrocarbon radical;

W = optionally substituted at least 1-18C monovalent hydrocarbon radical;

R8 = optionally substituted monovalent hydrocarbon radical;
X1 = optionally substituted n-valent hydrocarbon bridging 2-40C radical;
R9 = 4-40C divalent hydrocarbon radical;
R10 = optionally substituted at least 1-24C monovalent hydrocarbon radical;
a, b = 0-6.
The sum of a and b is 2-6 and n is the sum of a and b.
Preferred Solvents: The nonpolar reaction solvent(s) and nonpolar extraction solvent(s) are (cyclo)alkanes, alkenes, alkadienes, aldehydes, ketones, ethers, esters, amines, aromatics, silanes, silicones, and carbon dioxide. They are preferably (2,2-dimethyl)propane, (2,2-dimethyl)butane, isopropyl ether, triethylamine, heptane, octane, nonane, isobutyl isobutyrate, tributylamine, (un)decane, 2,2,4-trimethylpentyl acetate, isobutyl heptyl ketone, diisobutyl ketone, (cyclo)pentane, (cyclo)hexane, isobutylbenzene, n-nonylbenzene, n-octylbenzene, n-butylbenzene, p-xylene, ethylbenzene, 1,3,5-trimethylbenzene, m-xylene, toluene, o-xylene, (do)decene, tetradecene, **butadiene**, and/or heptadecanal. The polar reaction solvent(s) and polar extraction solvent(s) are nitriles, lactones, **alkanols**, cyclic acetals, pyrrolidones, formamides, sulfoxides, and water. They are preferably propionitrile, 1,3-dioxolane, 3-methoxypropionitrile, 1-methyl-2-pyrrolidinone, N,N-dimethylformamide, 2-methyl-2-oxazoline, adiponitrile, acetonitrile, epsilon caprolactone, glutaronitrile, 3-methyl-2-oxazolidinone,dimethyl sulfoxide, sulfolane, and water.
Preferred Reactants: The reactants comprise alkadiene(s) and unsaturated **alcohol**(s).
Preferred Product: The products comprise unsaturated **alcohol**(s) and hydroxyaldehyde(s).

TECHNOLOGY FOCUS - CHEMICAL ENGINEERING - Preferred Device: The separation zone comprises vaporizer(s), distillation column(s), and fractional countercurrent extractor(s). Preferred Mechanism: The reaction product fluid first passes through a vaporizer or distillation column to remove at least some products, reaction byproducts and unreacted reactants and the resulting reaction product fluid, depleted in products, reaction byproducts and unreacted reactants, then passes to a fractional countercurrent extractor.

L8 ANSWER 7 OF 20 WPIDS (C) 2003 THOMSON DERWENT
AN 2001-616275 [71] WPIDS
DNC C2001-184488
TI Separation of products from reaction product fluid by fractional countercurrent extraction, involves subjecting reaction fluid to extraction with immiscible solvents to separate into polar and non-polar phases.
DC E11 J01 J04
IN ARGYROPOULOS, J N; BRIGGS, J R; BRYANT, D R; KANEL, J S; LEE, M M; MAHER, J M; PHILLIPS, A G; ROESCH, B M
PA (UNIC) UNION CARBIDE CHEM & PLASTICS TECHNOLOGY
CYC 91
PI WO 2001068248 A2 20010920 (200171)* EN 64p
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ NL OA PT SD SE SL SZ TR TZ UG ZW
W: AE AL AM AT AU AZ BA BB BG BR BY CA CH CN CR CU CZ DE DK DM EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX NO NZ PL PT RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG UZ VN YU ZA ZW
US 6294700 B1 20010925 (200171)

AU 2001053851 A 20010924 (200208)
ADT WO 2001068248 A2 WO 2001-US40287 20010314; US 6294700 B1 US 2000-526636 20000315; AU 2001053851 A AU 2001-53851 20010314
FDT AU 2001053851 A Based on WO 200168248
PRAI US 2000-526636 20000315
AB WO 200168248 A UPAB: 20011203
NOVELTY - Separation of products from reaction product fluid involves subjecting fluid having metal-organophosphorous ligand complex **catalyst**, optionally free organophosphorous ligand and products, to fractional countercurrent extraction with immiscible solvents, to separate into polar and non-polar phases.

DETAILED DESCRIPTION - Separation of one or more products from a reaction product fluid involves subjecting reaction product fluid to fractional countercurrent extraction with two or more immiscible extraction solvents, to obtain polar and non-polar phase. The non-polar phase is then recovered from polar phase. The reaction product fluid comprises metal-organophosphorous ligand complex **catalyst**, optionally free organophosphorous ligand, one or more polar and non-polar reaction solvents. The immiscible extraction solvent comprises one or more polar and non-polar extraction solvents. The polar phase comprises metal-organophosphorous ligand complex **catalyst**, optionally free organophosphorous ligand, polar reaction solvents, and polar extraction solvents. The non-polar phase comprises one or more products, and one or more non-polar reaction solvents, and non-polar extraction solvents. The organophosphorous ligand has partition coefficient (Kp1) of more than 5, between polar and non-polar phases. Partition coefficient (Kp1) is the ratio of concentration of organophosphorous ligand in the polar phase after extraction to the concentration of organophosphorous ligand in the non-polar phase after extraction. One or more products have partition coefficient (Kp2) of less than 2, between polar and non-polar phases. Partition coefficient (Kp2) is the ratio of concentration of products in the polar phase after extraction to the concentration of products in the non-polar phase after extraction. INDEPENDENT CLAIMS are also included for the following:

(i) producing one or more products, which involves reacting one or more reactants in presence of a metal-organophosphorous ligand complex **catalyst**, optionally free organophosphorous ligand, one or more polar reaction solvents, and non-polar reaction solvents, to form a reaction product fluid; and

(ii) a reaction mixture comprising one or more products.

USE - For separating one or more products from reaction product fluid containing metal-organophosphorous ligand complex **catalyst**, optionally free organophosphorous ligand, products, organophosphorous ligand degradation products, reaction byproducts, polar reaction solvents, and non-polar solvents by fractional countercurrent extraction (claimed).

ADVANTAGE - The desired product along with **phosphorus** ligand degradation products and reaction byproducts, can be separated from the reaction product fluid without using vaporization separation process, and harsh conditions associated with the process. Degradation of organophosphorous ligand and deactivation of **catalyst** are prevented and/or lessened. The build up of organophosphorous ligand degradation products and reaction byproducts in the reaction product fluid are prevented. Hence, decrease in **catalyst** efficiency, raw material conversion, and product selectivity are prevented.

DESCRIPTION OF DRAWING(S) - The figure shows the schematic block diagram of fractional countercurrent extractor.

Dwg.1/1
TECH UPTX: 20011203

TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preferred Process: The reaction product fluid is formed by hydroacylation (intramolecular and intermolecular), hydrocyanation, hydroamidation, hydroesterification, aminolysis, **alcoholysis**, hydrocarbonylation, (reductive) hydroformylation, hydrogenation, oligomerization, (hydroxy) **carbonylation**, isomerization or transfer hydrogenation process. The derivatives of one or more products is obtained by hydrogenation, esterification, etherification, amination, alkylation, dehydrogenation, reduction, acylation, condensation, carboxylation, **carbonylation**, oxidation, cyclization, reductive amination, silylation, hydrolysis, and (co) polymerization. Preferred Solvents: The polar reaction solvents and polar extraction solvents are same or different, and are selected from nitriles, lactones, **alkanols**, cyclic acetals, pyrrolidones, formamides, sulfoxides and water, preferably propionitrile, 1,3-dioxolane, 3-methoxypropionitrile, 1-methyl-2-pyrrolidinone, N,N-dimethylformamide, 2-methyl-2-oxazoline, adiponitrile, acetonitrile, epsilon-caprolactone, glutaronitrile, 3-methyl-2-oxazolidinone, dimethyl sulfoxide, sulfolane, and water. The non-polar reaction solvents and non-polar extraction solvents are alkanes, cycloalkanes, alkenes, alkadienes, aldehydes, ketones, ethers, esters, amines, aromatics, silanes, silicones, and carbon dioxide, preferably propane, 2,2-dimethylpropane, butane, 2,2-dimethylbutane, pentane, isopropyl ether, hexane, triethylamine, heptane, octane, nonane, decane, isobutyl isobutyrate, tributylamine, undecane, 2,2,4-trimethylpentyl acetate, isobutyl heptyl ketone, diisobutyl ketone, cyclopentane, cyclohexane, isobutylbenzene, n-nonylbenzene, n-octylbenzene, n-butylbenzene, p-xylene, ethylbenzene, 1,3,5-trimethylbenzene, m-xylene, toluene, o-xylene, decene, dodecene, tetradecene, **butadiene**, and heptadecanal.

Preferred **Catalyst**: The metal-organophosphorous ligand complex **catalyst** comprises rhodium complexed with an organophosphorous ligand. The organophosphorous ligand is a triorganophosphine ligand of formula (I), a monoorganophosphite of formula (II), a diorganophosphite of formula (III), a triorganophosphite of formula (IV), or an organopolyphosphite containing two or more tertiary (trivalent) **phosphorus** atoms, of formula (V).

R1 = optionally substituted 1-24C or more monovalent hydrocarbon radical;
R3 = optionally substituted 4-40C or more trivalent hydrocarbon radical;
R4 = optionally substituted 4-40C or more divalent hydrocarbon radical;
W = optionally substituted 1-18C or more monovalent hydrocarbon radical;
R8 = optionally substituted monovalent hydrocarbon radical;
X1 = optionally substituted n-valent 2-40C hydrocarbon bridging radical;
R9 = divalent 4-40C hydrocarbon radical;
R10 = optionally substituted monovalent 1-24C hydrocarbon radical;
a,b = 0-6;
a+b = 2-6;
n = a+b.

TECHNOLOGY FOCUS - CHEMICAL ENGINEERING - Preferred Process: The reaction product fluid comprising one or more unreacted reactants, organophosphorous ligand degradation products, and reaction byproducts apart from other components, is supplied from the reaction zone to a separation zone. The separation zone comprises one or more vaporizers, distillation columns, and fractional countercurrent extractors, arranged in parallel or in series. In the separation zone, the reaction product fluid is initially passed through vaporizer, distillation column, or other separation apparatus, to remove some of the products, reaction byproducts and unreacted reactants, and the resulting reaction product fluid is then passed to a fractional countercurrent extractor for fractional countercurrent extraction. The polar phase further comprises one or more

unreacted reactants, and the non-polar phase further comprises one or more organophosphorous ligand degradation product, and reaction byproducts. The selectivity of polar phase for the organophosphorous ligand with respect to one or more products, is expressed by partition coefficient ratio (Ef1), which is the ratio of partition coefficient (Kp1) of organophosphorous ligand to the partition coefficient (Kp2) of one or more products. The value of Ef1 is more than 2.5, preferably more than 3. The value of Kp1 is more than 7.5, and value of Kp2 is less than 1.5. The selectivity of polar phase for organophosphorous ligand with respect to one or more organophosphorous ligand degradation products, is expressed by partition coefficient ratio (Ef2), which is the ratio of partition coefficient (Kp1) of organophosphorous ligand to the partition coefficient (Kp3) of one or more organophosphorous ligand degradation products. The partition coefficient (Kp3) is the ratio of concentration of organophosphorous ligand degradation products in the polar phase after extraction to the concentration of organophosphorous ligand degradation products in the non-polar phase after extraction. The value of Ef2 is more than 2.5, preferably more than 3. The selectivity of polar phase for organophosphorous ligand with respect to one or more reaction byproducts, is expressed by partition coefficient ratio (Ef3), which is the ratio of partition coefficient (Kp1) of organophosphorous ligand to the partition coefficient (Kp4) of one or more reaction byproducts. The partition coefficient (Kp4) is the ratio of concentration of reaction byproducts in the polar phase after extraction to the concentration of reaction byproducts in the non-polar phase after extraction. The value of Ef3 is more than 2.5.

L8 ANSWER 8 OF 20 WPIDS (C) 2003 THOMSON DERWENT
AN 2000-647138 [62] WPIDS
DNC C2000-195718
TI **Catalyst** for **carbonylation** of conjugated **dienes**, e.g. for production of dimethyl adipate and methyl pentenoate, comprises palladium cations and a bridged cyclic **phosphorus**-containing ligand.
DC A41 E17
IN DRENT, E; JAGER, W W
PA (SHEL) SHELL INT RES MIJ BV
CYC 92
PI WO 2000056695 A1 20000928 (200062)* EN 28p
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW NL OA PT SD SE SL SZ TZ UG ZW
W: AE AL AM AT AU AZ BA BB BG BR BY CA CH CN CR CU CZ DE DK DM DZ EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX NO NZ PL PT RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG US UZ VN YU ZA ZW
AU 2000032907 A 20001009 (200103)
BR 2000009187 A 20011226 (200206)
EP 1163202 A1 20011219 (200206) EN
R: AL AT BE CH CY DE DK ES FI FR GB GR IE IT LI LT LU LV MC MK NL PT RO SE SI
KR 2001112924 A 20011222 (200240)
CN 1344242 A 20020410 (200249)
JP 2002540091 W 20021126 (200307) 29p
AU 756055 B 20030102 (200319)
ADT WO 2000056695 A1 WO 2000-EP2375 20000316; AU 2000032907 A AU 2000-32907 20000316; BR 2000009187 A BR 2000-9187 20000316, WO 2000-EP2375 20000316; EP 1163202 A1 EP 2000-910854 20000316, WO 2000-EP2375 20000316; KR 2001112924 A KR 2001-712001 20010920; CN 1344242 A CN 2000-805356

20000316; JP 2002540091 W JP 2000-606559 20000316, WO 2000-EP2375 20000316; AU 756055 B AU 2000-32907 20000316

FDT AU 2000032907 A Based on WO 200056695; BR 2000009187 A Based on WO 200056695; EP 1163202 A1 Based on WO 200056695; JP 2002540091 W Based on WO 200056695; AU 756055 B Previous Publ. AU 200032907, Based on WO 200056695

PRAI EP 1999-302202 19990322

AB WO 200056695 A UPAB: 20001130

NOVELTY - A new **catalyst** system comprises:

(a) palladium cations,

(b) a **phosphorus**-containing ligand and

(c) anions.

The ligand comprises two 5- or more-membered cyclic groups each containing **phosphorus**, linked by a 1-4 atom organic group.

DETAILED DESCRIPTION - A new **catalyst** system comprises:

(a) palladium cations,

(b) a **phosphorus**-containing ligand of formula (I) and

(c) anions.

X1-R-X2 (I)

X1, X2 = cyclic groups with at least 5 ring atoms, one of which is P; and

R = a bivalent organic bridging group containing 1-4 bridge atoms.

One or both of X1 and X2 is/are substituted with 1-4C alkyl group(s).

INDEPENDENT CLAIMS are also included for:

(1) A process for the **carbonylation** of conjugated **dienes** by reaction with carbon monoxide and a hydroxyl group-containing compound in the presence of the **catalyst** (in which X1 and X2 need not be substituted).

(2) A process for preparing caprolactam, Nylon 6 or Nylon 6,6 using the **carbonylated diene** as intermediate.

USE - **Carbonylation catalyst**, especially for **carbonylation** of conjugated **dienes** (claimed). Useful reaction products include dimethyl adipate (intermediate for Nylon 6,6) and methyl pentenoate (intermediate for Nylon 6).

ADVANTAGE - The **catalyst** system has an unexpectedly high activity (allowing molar ratios of conjugated **diene** to palladium of well over 300:1) while still obtaining high selectivity. The presence of halides is not required, so allowing the use of cheaper types of reactor steel. Mono-esters and di-esters can be simultaneously produced.

Dwg.0/0

TECH UPTX: 20001130

TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preferred Ligand: The **phosphorus** ligand is especially 1,2-P,P'-bis(1,5-dimethyl, 9-phosphabicyclononyl)ethane.

Preferred **Catalyst**: Component (c) contains a protonic acid of pKa greater than 1 in aqueous solution at 25 deg.C (or its salt).

Preferred **Carbonylation** Process: The conjugated **diene** is 1,3-**butadiene**. The hydroxyl compound is a 1-6C **alkanol**.

L8 ANSWER 9 OF 20 WPIDS (C) 2003 THOMSON DERWENT

AN 2000-014411 [02] WPIDS

DNC C2000-003084

TI Oxidative **carbonylation** of **diene** compounds, useful for production of unsaturated acid esters from **butadiene** etc..

DC E17 J04

IN SCHAEFER, M; SCHULZ, M; SLANY, M

PA (BADI) BASF AG

CYC 21
PI DE 19822035 A1 19991118 (200002)* 5p
WO 9959718 A1 19991125 (200003) DE
RW: AT BE CH CY DE DK ES FI FR GB GR IE IT LU MC NL PT SE
W: JP KR US
EP 1083991 A1 20010321 (200117) DE
R: BE DE FR GB IT NL
JP 2002515463 W 20020528 (200238) 19p
ADT DE 19822035 A1 DE 1998-19822035 19980515; WO 9959718 A1 WO 1999-EP3187 19990510; EP 1083991 A1 EP 1999-923568 19990510, WO 1999-EP3187 19990510; JP 2002515463 W WO 1999-EP3187 19990510, JP 2000-549375 19990510
FDT EP 1083991 A1 Based on WO 9959718; JP 2002515463 W Based on WO 9959718
PRAI DE 1998-19822035 19980515
AB DE 19822035 A UPAB: 20000112
NOVELTY - A **catalyst** system containing subgroup 8 metal(s) or their compounds and a heteropolyacid of molybdenum, tungsten and/or vanadium in a molar excess (based on metal) of at least 2 is used for the oxidative **carbonylation** of **dienes**.
DETAILED DESCRIPTION - A process for the oxidative **carbonylation** of **dienes** comprises reacting diolefin(s) with a prim., sec. or tert. **alcohol**, carbon monoxide and oxygen at above 40 deg. C in the presence of a **catalyst** system containing:
(a) subgroup 8 metal(s) or their compounds; and
(b) a heteropolyacid of formula (I) in a molar excess of at least 2 based on metal.
(H)8+a-n(XMo12-a-bWbVaO40)(H2O)y (I)
X = **phosphorus**, silicon, arsenic, germanium, titanium or zirconium;
n = 5 if X = P or As, or 4 if X = Si, Ge, Ti or Zr;
a = 0-4;
b = 0-12; and
y = 0-40
An INDEPENDENT CLAIM is also included for the **catalyst** system described above.
USE - For the production of unsaturated carboxylic acid esters, especially pentadiene-carboxylic acid esters, methoxypentenoic acid esters and dehydroadipic acid esters from **butadiene**.
ADVANTAGE - Enables the oxidative **carbonylation** of **dienes** with high catalytic activity under non-corrosive conditions and without using a water interceptor. Prior art **catalyst** systems form very corrosive mixtures (copper/halogen-based systems) and/or require more than one process stage (metal/quinone systems).
Dwg.0/0
TECH UPTX: 20000112
TECHNOLOGY FOCUS - INORGANIC CHEMISTRY - Preferred Components: **Catalyst** component (a) comprises palladium on a support or a Pd(II) compound. In component (b), X = P.
Preferred heteropolyacids are H3PMo12O14 and/or H4SiMo12O14 (sic).

TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preferred Materials: **Dienes** of formula R1CH=CR3-CR4=CHR2 are used, in which R1-R4 = H, halogen, 1-4C alkyl or 6C aryl. Suitable **alcohols** are 1-6C aliphatic **alcohols**. Suitable reaction solvents are the **alcohol** itself, benzonitrile, acetonitrile, isocyanates, isothiocyanates, pyridine, pyrimidine, quinoline or isoquinoline.
Preferred Process: The process is carried out with a partial pressure ratio (CO/O2) of (1:1)-(20:1).

L8 ANSWER 10 OF 20 WPIDS (C) 2003 THOMSON DERWENT
AN 1998-557303 [47] WPIDS
DNC C1998-166808
TI **Carbonylation catalyst** system - comprises palladium compound, acid and asymmetric bi dentate **phosphorus** ligand.
DC A23 E19 J04
IN AGTERBERG, F P W; BUIJSEN, P F A; OEVERING, H; SIELCKEN, O E; TOTH, I
PA (STAM) DSM NV
CYC 72
PI WO 9845040 A1 19981015 (199847)* EN 16p
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW NL OA PT SD SE SZ UG ZW
W: AL AU BA BB BG BR CA CN CU CZ EE GE HU ID IL IS JP KP KR LC LK LR LT LV MG MK MN MX NO NZ PL RO SG SI SK SL TR TT UA US UZ VN YU
AU 9867507 A 19981030 (199911)
EP 977628 A1 20000209 (200012) EN
R: DE FR NL
CN 1252015 A 20000503 (200036)
US 6232262 B1 20010515 (200129)
EP 977628 B1 20010620 (200136) EN
R: DE FR NL
DE 69800968 E 20010726 (200150)
JP 2001518833 W 20011016 (200176) 16p
ADT WO 9845040 A1 WO 1998-NL192 19980406; AU 9867507 A AU 1998-67507 19980406; EP 977628 A1 EP 1998-912812 19980406, WO 1998-NL192 19980406; CN 1252015 A CN 1998-803990 19980406; US 6232262 B1 US 1999-414087 19991007; EP 977628 B1 EP 1998-912812 19980406, WO 1998-NL192 19980406; DE 69800968 E DE 1998-600968 19980406, EP 1998-912812 19980406, WO 1998-NL192 19980406; JP 2001518833 W JP 1998-542626 19980406, WO 1998-NL192 19980406
FDT AU 9867507 A Based on WO 9845040; EP 977628 A1 Based on WO 9845040; EP 977628 B1 Based on WO 9845040; DE 69800968 E Based on EP 977628, Based on WO 9845040; JP 2001518833 W Based on WO 9845040
PRAI EP 1997-201038 19970407
AB WO 9845040 A UPAB: 19981203
A **catalyst** system comprises a palladium compound, an acid compound of pKa greater than 2 in water at 18 deg. C, and an asymmetric bidentate **phosphorus** ligand of the formula (I).

R1R2P-X-PR3R4 (I)

The -PR1R2 group is different from the -PR3R4 group and X is a divalent organic group such that the shortest link between the two P atoms is a 2-10C chain optionally containing a S or O atom.

USE - The **catalyst** system is used for the **carbonylation** reaction of an olefinic compound, e.g. **butadiene** or an alkoxy-butene, carbon monoxide and optionally a co-reactant such as a 1-20C **alcohol**.

Dwg.0/0

L8 ANSWER 11 OF 20 WPIDS (C) 2003 THOMSON DERWENT
AN 1997-341271 [31] WPIDS
CR 1997-319699 [29]; 1997-319700 [29]; 1997-319701 [29]; 1997-319702 [29]; 1997-319703 [29]; 1997-319704 [29]; 1997-319705 [29]; 1997-332453 [30]; 1997-332454 [30]; 1999-166106 [14]; 1999-166107 [14]; 1999-166108 [14]; 1999-166109 [14]; 1999-166110 [14]; 1999-166111 [14]; 1999-166112 [14]; 1999-180082 [15]; 1999-213404 [18]; 1999-228626 [19]; 1999-253944 [21]; 1999-403822 [34]
DNC C1997-109553
TI Multistage reactor process, especially for hydroformylation - comprising

reaction of reactants with carbon mon oxide in the presence of metal-organo **phosphorus** ligand complex **catalyst**.

DC B05 E19 J04

IN BECKER, M C; BILLIG, E; BRYANT, D R; BUNNING, D L; NICHOLSON, J C

PA (UNIC) UNION CARBIDE CHEM & PLASTICS TECHNOLOGY

CYC 66

PI WO 9720793 A1 19970612 (199731)* EN 79p
RW: AT BE CH DE DK EA ES FI FR GB GR IE IT KE LS LU MC MW NL OA PT SD SE SZ UG
W: AL AM AU BB BG BR CA CN CZ EE GE HU IS JP KG KP KR LK LR LT LV MD MG MK MN MX NO NZ PL RO SG SI SK TR TT UA UZ VN
AU 9711292 A 19970627 (199742)
US 5728893 A 19980317 (199818) 24p
ZA 9610306 A 19981125 (199901) 77p
BR 9611830 A 19990309 (199916)
CZ 9801755 A3 19990317 (199917)
EP 904259 A1 19990331 (199917) EN
R: BE DE ES FR GB IT NL RO SE
CN 1203578 A 19981230 (199920)
MX 9804284 A1 19981001 (200019)
AU 719870 B 20000518 (200032)
TW 372950 A 19991101 (200036)
JP 2002515028 W 20020521 (200236) 66p
MX 203408 B 20010801 (200238)
EP 904259 B1 20020612 (200239) EN
R: BE DE ES FR GB IT NL RO SE
DE 69621839 E 20020718 (200255)
ES 2174125 T3 20021101 (200279)

ADT WO 9720793 A1 WO 1996-US19313 19961205; AU 9711292 A AU 1997-11292 19961205; US 5728893 A Provisional US 1995-8284P 19951206, Provisional US 1995-8286P 19951206, Provisional US 1995-8289P 19951206, Provisional US 1995-8763P 19951206, US 1996-757743 19961126; ZA 9610306 A ZA 1996-10306 19961206; BR 9611830 A BR 1996-11830 19961205, WO 1996-US19313 19961205; CZ 9801755 A3 WO 1996-US19313 19961205, CZ 1998-1755 19961205; EP 904259 A1 EP 1996-942139 19961205, WO 1996-US19313 19961205; CN 1203578 A CN 1996-198749 19961205; MX 9804284 A1 MX 1998-4284 19980529; AU 719870 B AU 1997-11292 19961205; TW 372950 A TW 1997-117740 19980728; JP 2002515028 W WO 1996-US19313 19961205, JP 1997-521398 19961205; MX 203408 B MX 1998-4284 19980529; EP 904259 B1 EP 1996-942139 19961205, WO 1996-US19313 19961205; DE 69621839 E DE 1996-621839 19961205, EP 1996-942139 19961205, WO 1996-US19313 19961205; ES 2174125 T3 EP 1996-942139 19961205

FDT AU 9711292 A Based on WO 9720793; BR 9611830 A Based on WO 9720793; CZ 9801755 A3 Based on WO 9720793; EP 904259 A1 Based on WO 9720793; AU 719870 B Previous Publ. AU 9711292, Based on WO 9720793; JP 2002515028 W Based on WO 9720793; EP 904259 B1 Based on WO 9720793; DE 69621839 E Based on EP 904259, Based on WO 9720793; ES 2174125 T3 Based on EP 904259

PRAI US 1996-757743 19961126; US 1995-8284P 19951206; US 1995-8286P 19951206; US 1995-8289P 19951206; US 1995-8763P 19951206

AB WO 9720793 A UPAB: 20021209
Processes using a reactor having more then 1 reactive stage comprises reacting 1 or more reactants with carbon monoxide in the presence of a metal-organo-**phosphorus** ligand complex **catalyst** and optionally free organo-**phosphorus** ligand, wherein the metal-organo-**phosphorus** ligand complex **catalyst**: (i) does not undergo deactivation in the presence of carbon monoxide alone; and/or (ii) effects a change in normal product selectivity of less than 0.2% normal product/pound/square inch of carbon monoxide partial pressure; and/or (iii) effects a change in reaction rate of less than

2%/pound/square inch of carbon monoxide partial pressure.

USE - The process is especially for hydroformylation for producing aldehydes by reacting olefinic unsaturated compounds with carbon monoxide and hydrogen in the presence of the above **catalyst** components (claimed). The apparatus can also be used for hydro-acylation (intramolecular and intermolecular), hydro-amidation, hydroesterification or **carbonylation** (claimed).

The hydroformylation processes can be asymmetric or non-asymmetric, especially for the production of non-optically active aldehydes, by hydroformylating 2-30C (preferably 4-20C) achiral alpha -olefins and/or achiral internal olefins, e.g. ethylene, propylene, 1-butene, 1-pentene, 1-hexene, styrene, **dienes**, alkyl alkenoates, alkenyl alkanoates, alkenyl alkyl ethers, alkenols, alkenals, vinyl acetate, methyl methacrylate, vinyl ethyl ether, 3-butenenitrile, 5-hexanamide, cyclooctadiene, camphene and linalool.

Non-optically active aldehyde products include, e.g. propionaldehyde, n-butyraldehyde, isobutyraldehyde, 2-, 3- and 4-pentenal, alkyl 5-formylvalerate, 2-methyl-1-nonanal, undecanal, 2-methyl-1-decanal and 2-methyl-1-triacontanal.

Optically active aldehyde products including (enantiomeric) aldehyde compounds are, e.g. S-2-(p-isobutylphenyl)-, S-2-(6-methoxy-2-naphthyl)-, S-2-(3-benzoylphenyl)-, S-2-(p-thienoylphenyl)-, S-2-(3-fluoro-4-phenyl)phenyl- or S-2-(4-(1,3-dihydro-1-oxo-2H-isoindol-2-yl)phenyl)-propionaldehydes or S-2-(2-methylacetaldehyde)-5-benzoyl-thiophene.

ADVANTAGE - The process provides high raw material conversion and/or reduced total reactor volume, reduced consumption of valuable **catalyst**, reduced formation of heavy by-products, elimination of expensive and complicated equipment for olefin recovery and recycle equipment and ability to use less pure feedstocks directly and efficiently. Heat of reaction can be removed both by an external heat exchanger and by internal cooling coils because of the changing heat loads in the different reactor compartments. Multiple reactive stages within a single vessel is a cost effective way of using the reactor vessel volume and it reduces the number of vessels required. Using fewer vessels reduces the overall capital expenditure and maintenance costs.

Dwg.0/0

L8 ANSWER 12 OF 20 WPIDS (C) 2003 THOMSON DERWENT
AN 1997-332453 [30] WPIDS
CR 1997-319699 [29]; 1997-319700 [29]; 1997-319701 [29]; 1997-319702 [29]; 1997-319703 [29]; 1997-319704 [29]; 1997-319705 [29]; 1997-332454 [30]; 1997-341271 [31]; 1999-166106 [23]; 1999-166107 [23]; 1999-166108 [24]; 1999-166109 [30]; 1999-166110 [30]; 1999-166111 [30]; 1999-166112 [30]; 1999-180082 [15]; 1999-213404 [15]; 1999-228626 [19]; 1999-253944 [21]; 1999-403822 [32]
DNC C1997-106626
TI Processes for obtaining more than one product - comprise contacting reactants in presence of metal-organo- poly phosphite ligand complex **catalyst**, optionally free organo- poly phosphite ligand, and sterically-hindered organo-**phosphorus** ligand.
DC B05 E19 J04
IN BYANT, D R; LEUNG, T W; BRYANT, D R
PA (UNIC) UNION CARBIDE CHEM & PLASTICS TECHNOLOGY
CYC 65
PI WO 9720795 A1 19970612 (199730)* EN 109p
RW: AT BE CH DE DK EA ES FI FR GB GR IE IT KE LS LU MC MW NL OA PT SD SE SZ UG
W: AL AM AU BB BG BR CA CN CZ EE GE HU IS JP KG KP KR LK LR LT LV MD

MG MK MN MX NO NZ PL RO SG SI SK TR TT UA UZ VN

AU 9713295 A 19970627 (199742)
US 5741945 A 19980421 (199823) 32p
EP 874797 A1 19981104 (199848) EN
R: BE DE ES FR GB IT NL SE
CZ 9801754 A3 19981111 (199851)
ZA 9610308 A 19981125 (199901) 107p
BR 9611663 A 19990223 (199913)
SK 9800690 A3 19990312 (199919)
CN 1203580 A 19981230 (199920)
MX 9804494 A1 19981201 (200024)
AU 724425 B 20000921 (200050)
EP 874797 B1 20010207 (200109) EN
R: BE DE ES FR GB IT NL RO SE
DE 69611765 E 20010315 (200122)
ES 2155949 T3 20010601 (200137)
JP 2002504888 W 20020212 (200215) 93p

ADT WO 9720795 A1 WO 1996-US19373 19961205; AU 9713295 A AU 1997-13295 19961205; US 5741945 A Provisional US 1995-8284P 19951206, Provisional US 1995-8286P 19951206, Provisional US 1995-8289P 19951206, Provisional US 1995-8763P 19951206, US 1996-757741 19961126; EP 874797 A1 EP 1996-944758 19961205, WO 1996-US19373 19961205; CZ 9801754 A3 WO 1996-US19373 19961205, CZ 1998-1754 19961205; ZA 9610308 A ZA 1996-10308 19961206; BR 9611663 A BR 1996-11663 19961205, WO 1996-US19373 19961205; SK 9800690 A3 WO 1996-US19373 19961205, SK 1998-690 19961205; CN 1203580 A CN 1996-198762 19961205; MX 9804494 A1 MX 1998-4494 19980605; AU 724425 B AU 1997-13295 19961205; EP 874797 B1 EP 1996-944758 19961205, WO 1996-US19373 19961205; DE 69611765 E DE 1996-611765 19961205, EP 1996-944758 19961205, WO 1996-US19373 19961205; ES 2155949 T3 EP 1996-944758 19961205; JP 2002504888 W WO 1996-US19373 19961205, JP 1997-521424 19961205

FDT AU 9713295 A Based on WO 9720795; EP 874797 A1 Based on WO 9720795; CZ 9801754 A3 Based on WO 9720795; BR 9611663 A Based on WO 9720795; AU 724425 B Previous Publ. AU 9713295, Based on WO 9720795; EP 874797 B1 Based on WO 9720795; DE 69611765 E Based on EP 874797, Based on WO 9720795; ES 2155949 T3 Based on EP 874797; JP 2002504888 W Based on WO 9720795

PRAI US 1996-757741 19961126; US 1995-8284P 19951206; US 1995-8286P 19951206; US 1995-8289P 19951206; US 1995-8763P 19951206

AB WO 9720795 A UPAB: 20020306
Reaction process comprises reacting one or more reactants in the presence of a metal-organopolyphosphite ligand complex **catalyst** (I) and optionally a free organopolyphosphite ligand (II), and an amount of a sterically-hindered organophosphorus ligand (III) different from the ligand in (I), to produce one or more products. (III) (i) has a coordination strength with respect to the metal in (I) less than the coordination strength of the organopolyphosphite ligand; (ii) when complexed with the metal to form a metal-sterically-hindered organophosphorus ligand complex **catalyst**, provides a reaction rate of at least 25% of that provided by the organopolyphosphite ligand of (I); (iii) optionally has a coordination strength with respect to the metal of (I) greater than carbon monoxide; and (iv) optionally when complexed with the metal to form a metal-sterically-hindered organophosphorus ligand complex **catalyst**, provides a normal:branched product isomer ratio lower than that provided by the organopolyphosphite ligand of (I). Also claimed are (A) a method of monitoring organopolyphosphite ligand depletion in a process as above; (B) a reaction mixture comprising one or more products, where the reaction mixture is prepared by a process as above; (C) a batchwise or continuously

generated reaction mixture; (D) a **catalyst** precursor composition; and (E) an improved process comprising reacting in at least one reaction zone one or more reactants in the presence of (I) and optionally (II) to produce a reaction product fluid comprising one or more products; and separating in at least one separation zone or in the reaction zone(s), the product(s) from the reaction product fluid; the improvement comprising conducting the process in the presence of (III).

USE - The process is useful for monitoring organopolyphosphite ligand depletion in hydroformylation, hydro-acylation (intramolecular and intermolecular), hydrocyanation, hydro-amidation, hydroesterification, aminolysis, **alcoholysis**, **carbonylation**, isomerisation or transfer hydrogenation processes (claimed). The indicator ligands are particularly useful in hydroformylation processes for reacting one or more olefinic unsaturated compounds with carbon monoxide and hydrogen for the production of aldehydes. The hydroformylation processes can be asymmetric or non-asymmetric, especially for the production of non-optically active aldehydes, by hydroformylating 2-30C (preferably 4-20C) achiral alpha -olefins and/or achiral internal olefins, e.g. ethylene, propylene, 1-butene, 1-pentene, 1-hexene, styrene, **dienes**, alkyl alkenoates, alkenyl alkanoates, alkenyl alkyl ethers, alkenols, alkenals, vinyl acetate, methyl methacrylate, vinyl ethyl ether, 3-butenenitrile, 5-hexanamide, cyclooctadiene, camphene and linalool.

ADVANTAGE - The sterically hindered organophosphorus ligands can give indications that the organopolyphosphite concentration has reached a point where it needs to be increased, and they can also serve to protect the metal, e.g. rhodium, from becoming intractable by helping to keep it in solution when organopolyphosphite ligand concentration is depleted.
Dwg.0/0

L8 ANSWER 13 OF 20 WPIDS (C) 2003 THOMSON DERWENT
AN 1997-319701 [29] WPIDS
CR 1997-319699 [29]; 1997-319700 [29]; 1997-319702 [29]; 1997-319703 [29]; 1997-319704 [29]; 1997-319705 [29]; 1997-332453 [30]; 1997-332454 [30]; 1997-341271 [31]; 1999-166106 [23]; 1999-166107 [23]; 1999-166108 [24]; 1999-166109 [30]; 1999-166110 [30]; 1999-166111 [30]; 1999-166112 [30]; 1999-180082 [15]; 1999-213404 [15]; 1999-228626 [19]; 1999-253944 [21]; 1999-403822 [32]
DNC C1997-103236
TI Separating **phosphorus** acidic compounds from a reaction product fluid containing a metal-organophosphite ligand complex **catalyst** - by treatment with water, followed by an ion exchange resin, useful in hydroformylation reactions of unsaturated olefinic compounds to aldehyde.
DC A41 E17 E19 J04
IN BILLIG, E; BRYANT, D R; NICHOLSON, J C
PA (UNIC) UNION CARBIDE CHEM & PLASTICS TECHNOLOGY
CYC 65
PI WO 9720796 A1 19970612 (199729)* EN 111p
RW: AT BE CH DE DK EA ES FI FR GB GR IE IT KE LS LU MC MW NL OA PT SD SE SZ UG
W: AL AM AU BB BG BR CA CN CZ EE GE HU IS JP KG KP KR LK LR LT LV MD MG MK MN MX NO NZ PL RO SG SI SK TR TT UA UZ VN
AU 9712801 A 19970627 (199742)
CZ 9801751 A3 19981014 (199847)
EP 876322 A1 19981111 (199849) EN
R: BE DE ES FR GB IT NL SE SI
ZA 9610310 A 19981125 (199901) 110p
BR 9611776 A 19990223 (199913)
US 5763680 A 19980609 (199914) 33p

MX 9804489 A1 19981201 (200024)
AU 721638 B 20000713 (200039)
EP 876322 B1 20010711 (200140) EN
R: BE DE ES FR GB IT NL RO SE
JP 2002515859 W 20020528 (200238) 103p

ADT WO 9720796 A1 WO 1996-US19380 19961205; AU 9712801 A AU 1997-12801 19961205; CZ 9801751 A3 WO 1996-US19380 19961205, CZ 1998-1751 19961205; EP 876322 A1 EP 1996-943600 19961205, WO 1996-US19380 19961205; ZA 9610310 A ZA 1996-10310 19961206; BR 9611776 A BR 1996-11776 19961205, WO 1996-US19380 19961205; US 5763680 A Provisional US 1995-8284P 19951206, Provisional US 1995-8286P 19951206, Provisional US 1995-8289P 19951206, Provisional US 1995-8763P 19951206, US 1996-756788 19961126; MX 9804489 A1 MX 1998-4489 19980605; AU 721638 B AU 1997-12801 19961205; EP 876322 B1 EP 1996-943600 19961205, WO 1996-US19380 19961205; JP 2002515859 W WO 1996-US19380 19961205, JP 1997-521428 19961205

FDT AU 9712801 A Based on WO 9720796; CZ 9801751 A3 Based on WO 9720796; EP 876322 A1 Based on WO 9720796; BR 9611776 A Based on WO 9720796; AU 721638 B Previous Publ. AU 9712801, Based on WO 9720796; EP 876322 B1 Based on WO 9720796; JP 2002515859 W Based on WO 9720796

PRAI US 1995-8763P 19951206; US 1995-8284P 19951206; US 1995-8286P 19951206; US 1995-8289P 19951206; US 1996-756788 19961126; US 1996-757743 19961126

AB WO 9720796 A UPAB: 20020618

Separating one or more **phosphorous** acidic compounds from a reaction product fluid containing a metal-organophosphite ligand complex **catalyst** and optionally free organophosphite ligand, comprises: (a) treating the reaction product fluid with water to remove at least some of the **phosphorus** acidic compounds; and (b) treating the water from step (a) with a ion exchange resin to remove at least some of the **phosphorus** acidic compounds from the water.

Also claimed are: (i) stabilising organophosphite ligand against hydrolytic degradation and/or metal-organophosphite ligand complex **catalyst** against deactivation; and (ii) preventing and/or lessening hydrolytic degradation of organophosphite ligand.

USE - The process is useful for stabilising organophosphite ligands against hydrolytic degradation and deactivation in hydroformylation, hydroacylation (intramolecular and intermolecular), hydrocyanation, hydroamidation, hydroesterification, aminolysis, **alcoholysis**, **carbonylation**, isomerisation or transfer hydrogenation processes (claimed).

The hydroformylation processes can be asymmetric or non-asymmetric, especially for the production of non-optically active aldehydes, by hydroformylating 2-30C (preferable 4-20 deg. C) achiral alpha -olefins and/or chiral internal olefins, e.g. ethylene, propylene, 1-butene, 1-pentene, 1-hexene, styrene, **dienes**, alkyl alkenoates, alkenyl alkanoates, alkenyl alkyl ethers, alkenols, alkenals, vinyl acetate, methyl methacrylate, vinyl ethyl ether, 3-butenenitrile, 5-hexenamide, cyclooctadiene, camphene and linalool.

Prochiral and chiral olefins useful in asymmetric hydroformylation that can be used to produce enantiomeric aldehyde mixtures are, e.g. of formula: R1R2C=CR3R4; where R1,R2,R3 and R4 = hydrogen, alkyl, optionally substituted with dialkylamino, alkoxy, acyloxy, halo, nitro, nitrile, thio, carbonyl, carboxyamide, carboxaldehyde, carboxyl, carboxylic ester; aryl optionally substituted with alkyl, amino, alkylamino, dialkylamino, hydroxy, alkoxy, acyloxy, halo, nitrile, nitro, carboxyl, carboxaldehyde, carboxylic ester, carbonyl or thio; acyloxy; alkoxy; amino; acylamino; diacylamino; nitro; carbonyl; nitrile; carboxyl; carboxamide; carboxaldehyde; carboxylic ester' alkylmercaptan; and the R groups are

optionally connected to form ring compounds, e.g. 3-methyl-1-cyclohexene.
on-optically active aldehyde products include, e.g. propionaldehyde, n-butyraldehyde, isobutyraldehyde, 2-0, 3- or 4-pentenal, alkyl 5-formylvalerate, 2-methyl-1-nonanal, undecenal, 2-methyl 1-decanal and 2-methyl- 1-triacontanal. Optically active aldehyde products including (enantiomeric) aldehyde compounds are, e.g. S-2-(p-isobutylphenyl)-, S-2-(6-methoxy-2-naphthyl)-, -S-2-(3- benzoylphenyl)-, S2-(p-thenoylphenyl)- S-2-(3-fluoro-4- phenyl)phenyl- or S-2-(4-(1,3-dihydro-1-oxo-2H-isoindol-2- yl)phenyl)-propionaldehydes or S-2-(2-methylacetaldehyde)-5- benzoyl-thiophene.
ADVANTAGE - The loss of organophosphite ligand can be minimised and the water used to remove **phosphorous** acidic compounds can be treated with ion exchange resin at high temperatures.
Dwg.1/1

L8 ANSWER 14 OF 20 WPIDS (C) 2003 THOMSON DERWENT
AN 1995-404078 [51] WPIDS
DNC C1995-173555
TI Bidentate phosphine ligands, useful in olefin hydroformylation - contg. an ortho ring system with two aryl gps. connected to two bridges, the **phosphorous** atoms being connected to the aryl gps..
DC A12 E11 E19 J04
IN DE, VRIES J G; KAMER, P C J; KRANENBURG, M; VAN, LEEUWEN P W N; VAN, LEEUWEN P W N M
PA (STAM) DSM NV
CYC 64
PI WO 9530680 A1 19951116 (199551)* EN 44p
RW: AT BE CH DE DK ES FR GB GR IE IT KE LU MC MW NL OA PT SD SE SZ UG
W: AM AU BB BG BR BY CA CN CZ EE FI GE HU IS JP KG KP KR KZ LK LR LT LV MD MG MN MX NO NZ PL RO RU SG SI SK TJ TM TT UA US UZ VN
AU 9523753 A 19951129 (199609)
BE 1008343 A3 19960402 (199620) FR
EP 758338 A1 19970219 (199713) EN
R: BE DE ES FR GB IT NL
JP 09512817 W 19971222 (199810) 41p
KR 97702867 A 19970610 (199825)
US 5817848 A 19981006 (199847)
CN 1151745 A 19970611 (200132)
ADT WO 9530680 A1 WO 1995-NL161 19950504; AU 9523753 A AU 1995-23753 19950504; BE 1008343 A3 BE 1994-470 19940506; EP 758338 A1 EP 1995-916857 19950504, WO 1995-NL161 19950504; JP 09512817 W JP 1995-528856 19950504, WO 1995-NL161 19950504; KR 97702867 A WO 1995-NL161 19950504, KR 1996-706322 19961105; US 5817848 A US 1996-746189 19961106; CN 1151745 A CN 1995-193971 19950504
FDT AU 9523753 A Based on WO 9530680; EP 758338 A1 Based on WO 9530680; JP 09512817 W Based on WO 9530680; KR 97702867 A Based on WO 9530680
PRAI BE 1994-470 19940506
AB WO 9530680 A UPAB: 19951221
Bidentate phosphine ligands of formula (I) in which P-atoms are connected via a bridging gp. comprising an ortho-ring annular system made up of two aryl gps. connected to two bridges, a first bridge consisting of -O- or -S- and a second bridge being a gp. contg. O, S, N, Si, C or combinations; the P atom being connected to the aryl gps. of the bridge at the ortho position relative to the -O- or -S- atom of the first bridge, are new: X and Y are the first and second bridges, respectively; R10, R11, R12 and R13 = 1-14C organic gps.
USE - The ligands are useful for hydroformylation of 2-20C ethylenically unsatd. organic cpds., esp. for conversion of olefins to

aldehydes, including terminal aldehydes (claimed); and can also be used for hydrogenation; hydrocyanation of, e.g. ethylene, propylene, 1-butene, 2-octene, 3-pentenenitrile or 3-pentenoic acids; polymerisation; isomerisation; **carbonylation**; cross-coupling; and metathesis (claimed). Cpds. contg. functional gps., e.g. carboxylic acids, esters, amides, acrylamides, nitriles, aldehydes, ketones, **alcohols** and ethers can be hydroformylated; and unsatd. polymers, e.g. 1,2-polybutadiene can be converted to polymers with aldehyde gps. **Butadiene** is converted to a pentenoic ester (claimed).

ADVANTAGE - High catalytic activities are obtd. when the ligands are used with transition metals; 50% fewer by-prods. are formed; and the ligands are more stable in air and are storage stable, compared with prior art ligands. Remarkable resistance against oxidn. by HCN is obtd. when using the ligands with Ni(O), so that the **catalyst** remains active to the end of the reaction and high concns. of HCN can be used, leading to higher productivity. The ligands form complexes giving high turnover numbers in isomerisation reactions. Conversions of e.g. greater than 98%, selectivities to aldehydes of greater than 95% and selectivities to n-aldehydes of greater than 92% are obtd.

Dwg.0/4

L8 ANSWER 15 OF 20 WPIDS (C) 2003 THOMSON DERWENT
AN 1995-155183 [20] WPIDS
DNC C1995-071463
TI Prepn. of (opt. 2-substd.) 2-methyl-cyclopentanone - from **butadiene** and acyl-acetate or malonate, using rhodium-phosphine **catalyst**, etc., useful for synthesis of fungicides.
DC C03
IN BUFORN, A; CLAVEL, J; CROCHEMORE, M; BUFORM, A; CLAVEL, J L; BUFOM, A
PA (RHON) RHONE POULENC AGROCHIMIE; (RHON) RHONE-POULENC AGROCHIMIE
CYC 33
PI WO 9509830 A1 19950413 (199520)* FR 36p
RW: AT BE CH DE DK ES FR GB GR IE IT LU MC NL PT SE
W: AU BR BY CA CN CZ FI HU JP KR KZ RU SI UA US
FR 2710908 A1 19950414 (199520)
AU 9479958 A 19950501 (199532)
ZA 9407879 A 19950726 (199536) 48p
EP 722432 A1 19960724 (199634) FR
R: AT BE CH DE DK ES FR GB GR IE IT LI LU MC NL PT SE
FI 9601553 A 19960409 (199636)
CZ 9601007 A3 19960717 (199637)
AU 675367 B 19970130 (199713)
BR 9407734 A 19970211 (199713)
JP 09503219 W 19970331 (199723) 36p
HU 74481 T 19970128 (199746)
CN 1132503 A 19961002 (199802)
ADT WO 9509830 A1 WO 1994-FR1157 19941004; FR 2710908 A1 FR 1993-12153 19931007; AU 9479958 A AU 1994-79958 19941004; ZA 9407879 A ZA 1994-7879 19941007; EP 722432 A1 EP 1994-931058 19941004, WO 1994-FR1157 19941004; FI 9601553 A WO 1994-FR1157 19941004, FI 1996-1553 19960409; CZ 9601007 A3 CZ 1996-1007 19941004; AU 675367 B AU 1994-79958 19941004; BR 9407734 A BR 1994-7734 19941004, WO 1994-FR1157 19941004; JP 09503219 W WO 1994-FR1157 19941004, JP 1995-510645 19941004; HU 74481 T WO 1994-FR1157 19941004, HU 1996-905 19941004; CN 1132503 A CN 1994-193694 19941004
FDT AU 9479958 A Based on WO 9509830; EP 722432 A1 Based on WO 9509830; AU 675367 B Previous Publ. AU 9479958, Based on WO 9509830; BR 9407734 A Based on WO 9509830; JP 09503219 W Based on WO 9509830; HU 74481 T Based on WO 9509830

PRAI FR 1993-12153 19931007
AB WO 9509830 A UPAB: 19950530
Prepn. of mono- or di-substd. cyclo-pentanones of formula (I) comprises the 4 stages, (a)-(d), which may all be effected in the same reactor. Stage (a) comprises reacting a 1,3 **butadiene** of formula CH2=C(R1)-CH=CH2 (II) with a cpd. with an active methylene gp. of formula XCOCH2COOR5(III) in the presence of a **catalyst** comprising a water soluble phosphine and at least one Rh cpd. giving a prod. of formula (IV); then sepn. of the prod. (in the organic phase) from the aq. **catalyst** phase and opt. purification by solvent extraction and/or distillation. Stage (b) comprises formation of the carboxylic acid of formula (VI) by (b1) decarboxylation of COX (when X = R6) with **alcoholic** alkali metal **alcoholate**, alkaline hydrolysis of the -COOR5 gp. and acidification; or (b2) (when X = OR6) by alkaline hydrolysis of COOR5 and COOR6, thermal decarboxylation and acidification; followed by isolation of (VI) (in the aq. phase) by sepn. from the organic phase and (opt) purification by solvent extraction. Stage (c) comprises hydroxy-**carbonylation** of (VI) using water with a mineral or organic acid **catalyst** and formic acid (as a source of CO) or 1-10MPa of CO to give a prod. of formula (VII), and isolation by precipitation with water, then opt. recrystallisation. Stage (d) comprises producing (I) by cyclising (VII) to the cyclic anhydride by reacting with a lower anhydride followed by loss of CO2 to give cpd. (I); or liq. or vapour phase pyrolysis of (VII) in the presence of a **catalyst** (VIIA); followed by isolating (I). (VIIA) is Rb, Cs, V, Mo, B, Al, Ga, In, Tl, Sn, Sb or Bi, or a deriv. of these; or opt. condensed **phosphoric** acid with the protons substd. by a metallic cation other than a metal from (i) or NH4+. R1 = H, 1-4C alkyl, 1-4C alkoxy or (R2)pR(CR3R4)q; R2 = 1-3C alkyl; R3, R4 = H or 1-3C alkyl; R = phenyl; p,q = 0-3; X = OR6 or OR6; R5, R6 = 1-6C alkyl.

USE - (I) are useful intermediates in the synthesis of benzylidene-azolylmethylcycloalkane fungicides.

ADVANTAGE - The method of prepn. uses easily accessible starting prods. and gives excellent productivities. It is easily carried out on an industrial scale and is partic. suited to prepn. of 2,2-dimethyl-cyclopentanone.

Dwg.0/0

L8 ANSWER 16 OF 20 WPIDS (C) 2003 THOMSON DERWENT
AN 1990-211885 [28] WPIDS
DNC C1990-091471
TI **Carbonylation** process of **diene**(s) - in presence of di carboxylic acids or di ol(s) and **catalyst** system.
DC A23 E11 E12 G02 G03
IN BREED, A J M; DRENT, E
PA (SHEL) SHELL INT RES MIJ BV; (SHEL) SHELL OIL CO
CYC 2
PI GB 2226822 A 19900711 (199028)*
US 5025092 A 19910618 (199127)
US 5128438 A 19920707 (199230) 4p
ADT GB 2226822 A GB 1988-30334 19881229; US 5025092 A US 1989-451920 19891218; US 5128438 A Div ex US 1989-451920 19891218, US 1991-680447 19910404
FDT US 5128438 A Div ex US 5025092
PRAI GB 1988-30334 19881229
AB GB 2226822 A UPAB: 19930928
Prepn of polyesters or polyanhydrides comprises reaction of (i) opt substd alkenols in which the OH gp is more than 4C atoms remote from the nearest C atom participating in the double bond; or (ii) opt substd alkenoic acids

in which the carboxyl is more than 3C atoms remote from the nearest C atom participating in the double bond, with CO in the absence of water and in the presence of a **catalyst** system obtd by combining (a) a Pd (II) cpd; (b) a monodentate organic phosphine and/or organic arsine and/or organic stilbene opt mixed with a bidentate phosphine, arsine or stilbene; and (c) a protonic acid, having a pka less than2 (measured at 18 deg C in aq soln) in which the mol ratio of (b) per gram atom of Pd is greater than 10 (pref 15-100), the mol ratio (b) to (c) is greater than 1 (pref greater than 2) and the reaction temp applied is less than 140 deg C (pref 60-130 deg C).

USE/ADVANTAGE - The process is efficient and economical having high selectivity to the desired prods which are suitable for viscosifiers, constituents of sealants, adhesives, paints, and in technical polymer compsns opt mixed with other polymers.

0/0

L8 ANSWER 17 OF 20 WPIDS (C) 2003 THOMSON DERWENT
AN 1988-272638 [39] WPIDS
DNC C1988-121319
TI Adipic acid di ester prepn. from 1,3-**butadiene** - by two-stage **carbonylation**, using palladium cpd. and poly dentate ligand contg. **phosphorus**, arsenic or antimony as **catalyst**.
DC A41 E17
IN DRENT, E; VAN, GOGH J; VANGOGH, J
PA (SHEL) SHELL CANADA LTD; (SHEL) SHELL INT RES MIJ BV
CYC 13
PI EP 284170 A 19880928 (198839)* EN 12p
R: AT BE DE FR GB IT NL
AU 8813568 A 19880929 (198847)
JP 63255245 A 19881021 (198848)
CN 88101605 A 19881123 (198944)
US 4861912 A 19890829 (198944) 8p
EP 284170 B 19911016 (199142)
R: AT BE DE FR GB IT NL
DE 3865474 G 19911121 (199148)
CA 1310664 C 19921124 (199301)
JP 2683621 B2 19971203 (199802) 9p
KR 141253 B1 19980701 (200017)
ADT EP 284170 A EP 1988-200578 19880325; JP 63255245 A JP 1988-68368 19880324; US 4861912 A US 1988-169698 19880318; CA 1310664 C CA 1988-561021 19880310; JP 2683621 B2 JP 1988-68368 19880324; KR 141253 B1 KR 1988-3128 19880323
FDT JP 2683621 B2 Previous Publ. JP 63255245
PRAI GB 1987-7405 19870327
AB EP 284170 A UPAB: 19930923

A new prepn. of adipic acid diesters, of general formula (I). The process is by three steps, comprising: (1) contacting 1,3-**butadiene** with CO and a cpd. of formula ZOH (II) in the presence of a **carbonylation catalyst** prepd. by combining a Pd cpd. with a polydentate ligand of formula (III), where M = a gp. 5a element of atomic number 15-51; R = a 2-6C divalent organic bridging gp. in which there are no substits. which could cause steric hindrance; R1, R2, R3 and R4 each = an optionally substd. hydrocarbon gp. and Z = H or a hydrocarbon gp. A cpd. of formula (IV) is formed. (2) Isolating cpd. (IV) from the reaction mixt. (3) Reacting cpd. (IV) with CO in the presence of a second **carbonylation catalyst**.

USE/ADVANTAGE - The prepn. is partic. for commercially important dimethyl adipate and overcomes previous problems of extremely high

pressures.
0/0

L8 ANSWER 18 OF 20 WPIDS (C) 2003 THOMSON DERWENT
AN 1988-184469 [27] WPIDS
DNC C1988-082265
TI Selective prepn. of alkene carboxylic acid derivs. - using palladium cpd. and at least one multi-dentate organic **phosphorous** ligand.
DC E11 E17
IN DRENT, E
PA (SHEL) SHELL INT RES MIJ BV
CYC 13
PI EP 273489 A 19880706 (198827)* EN
R: AT BE DE FR GB IT NL
AU 8782201 A 19880616 (198832)
JP 63156745 A 19880629 (198832)
CN 87107325 A 19880622 (198928)
US 5028734 A 19910702 (199129) 7p
EP 273489 B 19910724 (199130)
R: AT BE DE FR GB IT NL
DE 3771686 G 19910829 (199136)
CA 1292475 C 19911126 (199203)
KR 9601890 B1 19960206 (199908)
JP 2867137 B2 19990308 (199915) 7p
ADT EP 273489 A EP 1987-202334 19871125; JP 63156745 A JP 1987-308829 19871208; US 5028734 A US 1989-303596 19890127; KR 9601890 B1 KR 1987-13964 19871208; JP 2867137 B2 JP 1987-308829 19871208
FDT JP 2867137 B2 Previous Publ. JP 63156745
PRAI NL 1986-3139 19861210
AB EP 273489 A UPAB: 19930923
Selective **carbonylation** of conjugated **dienes** in the presence of a hydroxyl gp. containing cpd such as water, **alcohol**, phenol or carboxylic acid in the liquid phase is carried out in the presence of a specific substantially nitrogen-containing base free **catalyst** system formed by the combination of a) a palladium cpd. b) at least one multi dentate organic **phosphorus** ligand and c) opt. a monodentate phosphine deriv.
Specifically the bidentate phosphine deriv is of formula (I) and a monodentate ligand of formula

L8 ANSWER 19 OF 20 WPIDS (C) 2003 THOMSON DERWENT
AN 1982-79479E [38] WPIDS
TI Alpha,beta unsatd. carboxylic mono ester prodn. by **carbonylating** olefin in presence of palladium **catalyst** and quat. onium salt
DC E17
IN JENCK, J
PA (RHON) RHONE POULENC IND
CYC 16
PI FR 2498594 A 19820730 (198238)* 37p
EP 60734 A 19820922 (198239) FR
R: AT BE CH DE FR GB IT LI LU NL SE
JP 57146738 A 19820910 (198242)
BR 8200332 A 19821123 (198301)
DD 201672 A 19830803 (198348)
US 4433164 A 19840221 (198410)
JP 59040382 B 19840929 (198443)
CA 1177492 A 19841106 (198449)
EP 60734 B 19850306 (198510) FR

R: AT BE CH DE FR GB IT LI LU NL SE
DE 3262481 G 19850411 (198516)
ADT EP 60734 A EP 1982-400023 19820108; JP 57146738 A JP 1982-7726 19820122; US 4433164 A US 1982-341101 19820120
PRAI FR 1981-1205 19810123
AB FR 2498594 A UPAB: 19930915
Prodn. of alpha,beta-unsatd. carboxylic esters (I) comprises **carbonylating** a conjugated **diene** with CO in presence of the appropriate **alcohol**, a hydrohalic acid and Pd **catalyst** (i.e. the metal, oxide, salt or complex in which the anion associated with the Pd cation is a hard or intermediate base) at 50-150 deg.C and 50-300 bars CO.

The improvement is that a quat. onium salt (A) of N, P or As having a hard or intermediate base as anion is also present. 16 cations for (A) are specified e.g. tetra (m)ethylammonium; tetrabutylphosphonium; methyltriphenyl-ammonium or -phosphonium; tetraphenylarsonium or bis (buten-2-yldimethyl ammonium)-1,3-propane. Suitable anions for (A) are phosphate, mono- or di-hydrogen phosphate, nitrate, sulphate, chloro or bromo.

Esp.used to prepare ethyl penten-3-oate (Ia) from **butadiene**. (I) are prepd. with high selectivity and improved **diene** conversion and the **catalyst** system is stable.

L8 ANSWER 20 OF 20 WPIDS (C) 2003 THOMSON DERWENT
AN 1980-73514C [42] WPIDS
TI **Catalyst** used in prepn. of unsaturated acids or ester(s) - comprises complex of palladium salt, ligand, and specified solvent.
DC E19
PA (TEXC) TEXACO DEV CORP
CYC 11
PI BE 883698 A 19801001 (198042)*
DE 3019958 A 19801217 (198101)
NL 8003217 A 19801209 (198102)
BR 8003108 A 19801222 (198103)
GB 2052293 A 19810128 (198105)
US 4246183 A 19810120 (198106)
JP 55164648 A 19801221 (198109)
FR 2458535 A 19810206 (198113)
ZA 8003067 A 19810824 (198143)
GB 2052293 B 19830427 (198317)
CA 1145319 A 19830426 (198320)
NL 178864 B 19860102 (198604)
IT 1150957 B 19861217 (198847)
PRAI US 1979-46747 19790608
AB BE 883698 A UPAB: 19930902
Process comprises heating a 4-8C conjugated aliphatic **diene** at 30-150 degrees C under pressure with CO and >=1 mol. per 2 mols **diene** of wawter or a 1-12C **alkanol** in the presence of a PD **catalyst**. The **catalyst** comprises at least one Pd salt, at least one tertiary Group VB donor ligand, particularly **phosphorus**, and at least one solvent from oxygen and/or sulphur heterocyclic cpds. and O and N contg. heterocyclic, and O, N and S contg. heterocyclic and a solvent contg. P and N.

Catalyst has better stability in a single stage dimerisation/**carbonylation**, it gives faster **carbonylation** and a better selectivity to the linear cpds. desired.

L14 ANSWER 1 OF 5 WPIDS (C) 2003 THOMSON DERWENT
AN 2001-425042 [45] WPIDS
DNC C2001-128533
TI Polymeric phosphite composition useful as **catalyst** e.g. for converting unsaturated organic compound to a nitrile comprises a combination of two compositions.
DC A18 A23 E19
IN GREENE, R N; KRISTJANSDOTTIR, S S; TAM, W
PA (GREE-I) GREENE R N; (KRIS-I) KRISTJANSDOTTIR S S; (TAMW-I) TAM W; (DUPO) DU PONT DE NEMOURS & CO E I
CYC 31
PI WO 2001021684 A1 20010329 (200145)* EN 48p
RW: AT BE CH CY DE DK ES FI FR GB GR IE IT LU MC NL PT SE
W: BR CA CN CZ ID JP KR MX PL SG SK
US 6284865 B1 20010904 (200154)
US 2001049431 A1 20011206 (200203)
BR 2000014478 A 20020618 (200249)
EP 1216268 A1 20020626 (200249) EN
R: AT BE CH CY DE DK ES FI FR GB GR IE IT LI LU MC NL PT SE
JP 2003510385 W 20030318 (200321) 67p
ADT WO 2001021684 A1 WO 2000-US25568 20000919; US 6284865 B1 US 1999-399261 19990920; US 2001049431 A1 Div ex US 1999-399261 19990920, US 2001-865942 20010525; BR 2000014478 A BR 2000-14478 20000919, WO 2000-US25568 20000919; EP 1216268 A1 EP 2000-963590 20000919, WO 2000-US25568 20000919; JP 2003510385 W WO 2000-US25568 20000919, JP 2001-525254 20000919
FDT BR 2000014478 A Based on WO 200121684; EP 1216268 A1 Based on WO 200121684; JP 2003510385 W Based on WO 200121684
PRAI US 1999-399261 19990920; US 2001-865942 20010525
AB WO 200121684 A UPAB: 20010813
NOVELTY - A polymeric composition comprises repeat units derived from either a carbonyl compound (A1), a monomer (A2) and **phosphorochloridite** (A3) and/or repeat units derived from **phosphorus** trichloride, polyhydric alcohol and an aromatic diol.
DETAILED DESCRIPTION - A polymeric composition (A) comprises repeat units derived from a carbonyl compound (A1), a monomer (A2) and **phosphorochloridite** (A3). (A1) is of formula (R1O2C)m(OH)-Ar1-(OH)CO2R1)m, (R1O2C)m(OH)-Ar2-A2- Ar2-(OH)(CO2R1)m and/or (R1O2C)m-Ar2-Ar2-(CO2R1)m. (A2) is polyhydric alcohol and/or amine. (A3) is of formula ClP(O-Ar'2-R2)2.
Ar1 = 6-40C phenylene, 12-40C biphenylene, 10-40C naphthylene and/or 20-40C binaphthylene;
Ar2 = 6-40C phenylene and/or 10-40C naphthylene;
Ar'2 = Ar2;
A2 = -C(R1)(R1), -O-, -N(R1)-, -S-, -S(O)2- and/or -S(O)-;
R1 = H, 1-12C (cyclo)alkyl and/or 6-20C aryl;
R2 = R1, acetal, ketal, -OR3, -CO2R3, F, Cl, -NO2, -SO3R3, -CN, perhaloalkyl, -S(O)R3, -S(O)2R3, -CHO, -C(O)R3, cyclic ether and/or A1Z;
A1 = 1-12C alkylene;
Z = -CO2R3, -CHO, -C(O)R3, -C(O)SR3, -SR3, -C(O)NR1R1, -OC(O)R3, -OC(O)OR3, -N=C(R1)R1, -C(R1)=NR1, -C(R1)=N-O-R1, -P(O)(OR3)(OR3), -S(O)2R3, -S(O)R3, -C(O)OC(O)R3, -NR3CO2R3, -NR3C(O)N(R1)R1, F, Cl, -NO2, -SO3R3 and/or -CN;
R3 = 1-12C (cyclo)alkyl and/or 6-20C aryl;
m = 1 - 2.
Ar'2 are optionally linked to each other directly or through A2. In

(A3) R2 is ortho to the oxygen attached to **phosphorus**.
INDEPENDENT CLAIMS are also included for the following:
(1) preparation of (A) involves contacting (A1) with (A2) to produce an intermediate, which is further contacted with (A3);
(2) a process (P1) comprises contacting an unsaturated compound with a fluid comprising hydrogen cyanide in the presence of a group VII metal or a Lewis acid.
USE - As **catalyst** e.g. for converting an unsaturated organic compound to a nitrile and isomerizing a nitrile.
ADVANTAGE - The solubility of the composition can be controlled by varying the molecular weight and degree of branching. The **catalyst** produced by the composition can be substantially recovered by filtration.
Dwg.0/0

TECH UPTX: 20010813
TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preferred Compounds: (A1) is of formula (Ia) or (Ib) (preferably dialkyl 2,2'-dihydroxyl-1,1'-binaphthalene-3,3'-dicarboxylate, dialkyl 2,2'-dihydroxyl-1,1'-biphenyl-3,3'-dicarboxylate, 2,2'-dihydroxy-biphenyl-3,3'-dicarboxylic acid and/or 2,2'-dihydroxy-1,1'-binaphthyl-3,3'-dicarboxylic acid).(A1) is blended with at least one second carbonyl compound. The second carbonyl compound is of formula (R1O2C)m-Ar1-(CO2R1)m, (R1O2C)m-A1-(CO2R1)m, (R1O2C)m-Ar2-A1-Ar2-(CO2R1)m, (R1O2C)m-Ar2-(O)-A1-(O)-Ar2-(CO2R1)m and/or (R1O2C)m-(A1-O)p-A1-(CO2R1)m (preferably terephthalic acid, isophthalic acid, phthalic acid, dimethyl isophthalate, dimethyl phthalate, dimethyl terephthalate and/or 1,3,5-benzenetricarboxylic acid). (B2) is dialcohol, trialcohol and/or tetraalcohol (preferably 6,6'-dihydroxy-4,4,4',7,7,7'-hexamethyl bis-2,2'-spirochroman, 2,2'-diallylbisphenol A, bisphenol A, 4,4'-(1-methylethylidene)bis(2-(1-methylpropyl)phenol), 4,4'-thiophenol, 4,4'-dihydroxydiphenylsulfone, 4,4'-sulfonylbis(2-methylphenol), bis(4-hydroxy-3-methylphenyl)sulfide, 2,2'-bis(4-hydroxy-3-methylphenyl)propane, 4,4'-ethylidenebis(2,5-dimethylphenol), 4,4'-propylidenebis(2,5-dimethylphenol), 4,4'-benzylidenebis(2,5-dimethylphenol), 4,4'-ethylidenebis(2-isopropyl-5-methylphenol), 5,5'-diethyl-2,2'-bis(2-hydroxyphenyl)-5,5'-oxydimethylenebis(1,3-dioxane), 1,3-bis(2-hydroxyphenoxy)propane, 1,6-hexanediyl bis(2-hydroxyphenylacetate) and/or 1,6-hexanediyl bis(3-(2-hydroxyphenyl)propanoate). (B3) is of formula (IIa), (IIb) and/or (IIc).
R4 = H, 1-12C (cyclo)alkyl, acetal, ketal, -OR3, -CO2R3, 6-20C aryl, -SiR3, -NO2, -SO3R3, -S(O)R3, -S(O)2R3, -CHO, -C(O)R3, -F, -Cl, -CN, -CF3, -C(O)N(R3)(R3) and/or -A1Z;
Z = -CO2R3, -CHO, -C(O)R3, -C(O)SR3, -SR3, -C(O)NR1R1, -OC(O)R3, -OC(O)OR3, -N=CR1R1, -C(R1)=NR1, -C(R1)=N-O-R1, -P(O)(OR3)(OR3), -S(O)2R3, -S(O)R3, -C(O)OC(O)R3, -NR3CO2R3, -NR3C(O)NR1R1, F, Cl, -NO2, -SO3R3 and/or -CN;
R5 = H, F, Cl, 1-12C (cyclo)alkyl, 6-20C aryl, -OR3, -CO2R3, -C(O)R3, -CHO, -CN and/or -CF3;
R6 and R7 = H, 1-12C (cyclo)alkyl and/or 6-20C aryl.
The unsaturated compound has 2-30C per molecule and is of formula R8CH=CH-CH=CR9, CH=CH-(CH2)x-R10 and/or CH3-(CH2)y-CH=CH-(CH2)x-R10 (preferably **butadiene**, 3-pentenenitrile, 4-pentenenitrile, **methyl** 3-**pentenoate**, **methyl** 4-**pentenoate** and/or **methyl** 2-**pentenoate**.
R8 and R9 = H and/or 1-3C alkyl;
R10 = H, CN, CO2R11 and/or 1-20C perfluoroalkyl;
y = 0 - 12;
x = either 0 - 12 if R10 is H, CO2R11 or perfluoroalkyl, or 1 - 12 if R10 is CN;
R11 = 1-12C (cyclo)alkyl and/or 6-20C aryl.

TECHNOLOGY FOCUS - POLYMERS - Preferred Composition: The composition additionally contains at least one group VIII metal and at least one Lewis acid. The composition also comprising repeating units derived from **phosphorus** trichloride (B1), polyhydric alcohol (B2) and an aromatic diol (B3);
Preparation: The polymeric composition is prepared by either contacting PCl3 with (B2) to obtain a **phosphorus** containing polymer and further contacting the polymer with (B3); or contacting N,N-dialkyl dichlorophosphoramidite with (B2) to obtain polymeric **phosphoramidite**, which is contacted with an acid to produce a **phosphorus**-containing polymer, which is further contacted with an aromatic diol.
Preferred Process: The first contacting is carried out at about 100 - 450 degreesC (preferably 180 - 270 degreesC) for 1 minute - 24 hours. The second contacting is carried out at about -50 - 150 degreesC (preferably -30 - 80 degreesC) for about 1 minute - 24 hours. The ratio of **phosphorochloridite** to the alcohol group of the intermediate is from 0.5:1 - 10:1 (preferably 1:1). The process is carried out in an organic base. In (P1) a diolefinic compound (preferably **butadiene**) is contacted with a fluid comprising hydrogen cyanide in presence of group VIII metal or Lewis acid to produce 2-alkyl-3-monoalkenenitrile (preferably 2-methyl-3-butenenitrile). 2-alkyl-3-monoalkenenitrile is further contacted with group VIII metal or Lewis acid.

TECHNOLOGY FOCUS - INORGANIC CHEMISTRY - The group VIII metal is nickel, palladium and/or cobalt. The Lewis acid is an inorganic or organometallic compound of scandium, titanium, vanadium, chromium, manganese, iron, cobalt, copper, zinc, boron, aluminum, yttrium, zirconium, niobium, molybdenum, cadmium, rhenium and/or tin (preferably zinc chloride, cadmium chloride, iron chloride, triphenyl boron, (C6H5)3SnCF3SO3, (C6H5)3SnCH3C6H5SO3 and/or (C6H5)3Sn(C6H5)3BCN.

L14 ANSWER 2 OF 5 WPIDS (C) 2003 THOMSON DERWENT
AN 2000-204497 [18] WPIDS
CR 1997-558503 [51]; 1999-180083 [15]
DNC C2000-062985
TI Preparation of terminal aldehydes, e.g. 5-formylvaleronitrile, by hydroformylation of ethylenically unsaturated compound in presence of iridium or rhodium and bidentate organic phosphate ligand **catalyst** system.
DC E11 E17 J04
IN BURKE, P M; GARNER, J M; HANSEN, C B; KREUTZER, K A; SNIJDER, C S; TAM, W; TEUNISSEN, A J J M
PA (STAM) DSM NV; (DUPO) DUPONT DE NEMOURS & CO E I
CYC 1
PI US 6018081 A 20000125 (200018)* 15p
ADT US 6018081 A CIP of US 1996-616721 19960315, US 1997-843130 19970428
PRAI US 1997-843130 19970428; US 1996-616721 19960315
AB US 6018081 A UPAB: 20001123
NOVELTY - Preparation of terminal aldehydes comprises hydroformylation of an ethylenically unsaturated compound with carbon monoxide and hydrogen in the presence of a **catalyst** system comprising iridium or rhodium and a bidentate organic phosphate ligand.
DETAILED DESCRIPTION - The bidentate organic phosphate ligand is of formula (I) in which the two **phosphorus** atoms of the phosphate ligand are linked with a 2,2'-dihydroxyl-1,1'-binapthalene bridging group (Q).

Q = formula (II) or (III);
R1 and R2 = substituents other than hydrogen;
R3 and R4 = substituted monovalent aryl and/or any one of OR3 and OR4 connected to one **phosphorus** atom forms an -O-R5-O-;
R5 = divalent organic group containing 1-2 aryl.
USE - The process is useful for preparation of, e.g. methyl-5-formylvalerate, 5-formylvaleronitrile (a precursor for caprolactam) and pentanal.
ADVANTAGE - High selectivities to terminal aldehyde compounds and high conversion, e.g. 84.9% and 97.5%, respectively (in examples), with high **catalyst** activity are obtained. In addition, the linearity of the product is high, e.g. 98.7% (in examples) allowing ease of isolation of the desired terminal aldehyde from a mixture of terminal and branched aldehydes.
Dwg.0/0

TECH UPTX: 20000412
TECHNOLOGY FOCUS - INORGANIC CHEMISTRY - The ethylenically unsaturated organic compound is 2-20C (preferably 1,3-**butadiene**, or a 4-20C internally ethylenically unsaturated organic compound, especially 3-pentenenitrile, 3-pentenoic acid or 1-6C alkyl 3-pentenoate ester, especially **methyl** 3-**pentenoate** or ethyl 3-pentenoate).
Preferred Conditions: The amount of rhodium is 10-10000 ppm. The ligand and rhodium are in a ratio of 1-10, the reaction is at 50-150 degreesC, the total pressure is 0.1-20 MPa, and the carbon monoxide and hydrogen are in a ratio of 0.1-10.

L14 ANSWER 3 OF 5 WPIDS (C) 2003 THOMSON DERWENT
AN 1998-481100 [41] WPIDS
DNC C1998-145605
TI Pentenoic acid derivative preparation - using a **catalyst** system comprising palladium, a **phosphorus** ligand and an acid promoter.
DC A41 E11 E17 J04
IN BURKE, P M; OEVERING, H; SIELCKEN, O E
PA (STAM) DSM NV
CYC 71
PI WO 9838151 A1 19980903 (199841)* EN 26p
RW: AT BE CH DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW NL OA PT SD SE SZ UG ZW
W: AL AU BA BB BG BR CA CN CU CZ EE GE HU ID IL IS JP KP KR LC LK LR LT LV MG MK MN MX NO NZ PL RO SG SI SK SL TR TT UA US UZ VN YU
AU 9855795 A 19980918 (199908)
EP 975574 A1 20000202 (200011) EN
R: BE DE ES FR GB IT NL
CN 1252786 A 20000510 (200036)
US 6175036 B1 20010116 (200106)
KR 2000075730 A 20001226 (200134)
JP 2001513103 W 20010828 (200156) 23p
ADT WO 9838151 A1 WO 1998-NL44 19980122; AU 9855795 A AU 1998-55795 19980122; EP 975574 A1 EP 1998-900779 19980122, WO 1998-NL44 19980122; CN 1252786 A CN 1998-804328 19980122; US 6175036 B1 Div ex US 1997-805829 19970226, US 1999-384060 19990826; KR 2000075730 A WO 1998-NL44 19980122, KR 1999-707799 19990826; JP 2001513103 W JP 1998-537536 19980122, WO 1998-NL44 19980122
FDT AU 9855795 A Based on WO 9838151; EP 975574 A1 Based on WO 9838151; KR 2000075730 A Based on WO 9838151; JP 2001513103 W Based on WO 9838151
PRAI US 1997-805829 19970226; US 1999-384060 19990826
AB WO 9838151 A UPAB: 19981014
Preparation of (1) an alkyl pentenoate or (2) an aryl pentenoate is

effected by contacting (1) an alkoxy-butene or (2) an aryloxy-butene with carbon monoxide in the presence of a **catalyst** system comprising palladium, a **phosphorus** ligand and an acid promoter. The molar ratio of (1) 3-alkoxy-1-butene:1-alkoxy-2-butene, or (2) 3-aryloxy-1-butene:1-aryloxy-2-butene is greater than 4.

Also claimed is the preparation of a pentenoic acid derivative starting from **butadiene**, carbon monoxide and a nucleophilic compound, ROH having a removable hydrogen atom and where R = 1-20C aliphatic, cycloaliphatic or aromatic group, using a **catalyst** system containing palladium and a phosphine ligand. The molar ratio of butene-1 derivative:butene-2 derivative is greater than 4.

USE - **Methyl** and ethyl **pentenoates** can be used as precursors in other processes, e.g. epsilon-caprolactam and adipic acid preparations.

ADVANTAGE - The rate of reaction in the preparation of alkyl or aryl pentenoate compounds and the selectivity to the pentenoate compounds is improved over previous methods. The reaction can be performed at a lower temperature and consequently the rate of consumption of the phosphine ligand/kg of pentenoic acid derivative is also lower. No, or only a small amount of halogens are used and weak acids can be used compared with the strong acids necessary in previous methods.

Dwg.0/0

L14 ANSWER 4 OF 5 WPIDS (C) 2003 THOMSON DERWENT
AN 1997-558503 [51] WPIDS
CR 1999-180083 [15]; 2000-204497 [12]
DNC C1997-178231
TI Terminal aldehyde compounds preparation - by hydroformylation of ethylenically unsaturated compound using **catalyst** system containing iridium or rhodium and bidentate organic phosphate ligand..
DC A41 E19 J04
IN BURKE, P M; GARNER, J M; HANSEN, C B; KREUTZER, K A; SNIJDER, C S; TAM, W; TEUNISSEN, A J J; TEUNISSEN, A J J M
PA (STAM) DSM NV; (DUPO) DU PONT DE NEMOURS & CO E I
CYC 67
PI WO 9733854 A1 19970918 (199751)* EN 46p
RW: AT BE CH DE DK EA ES FI FR GB GH GR IE IT KE LS LU MC MW NL OA PT SD SE SZ UG
W: AL AU BA BB BG BR CA CN CU CZ EE GE HU IL IS JP KP KR LC LK LR LT LV MG MK MN MX NO NZ PL RO SG SI SK TR TT UA UZ VN YU
AU 9720451 A 19971001 (199805)
EP 888274 A1 19990107 (199906) EN
R: BE DE ES FR GB IT NL
TW 343195 A 19981021 (199909)
CN 1224413 A 19990728 (199948)
JP 2000506525 W 20000530 (200033) 42p
EP 888274 B1 20000906 (200044) EN
R: BE DE ES FR GB IT NL
DE 69703035 E 20001012 (200059)
KR 99087823 A 19991227 (200059)
ES 2152085 T3 20010116 (200108)
ADT WO 9733854 A1 WO 1997-NL114 19970307; AU 9720451 A AU 1997-20451 19970307; EP 888274 A1 EP 1997-908575 19970307, WO 1997-NL114 19970307; TW 343195 A TW 1996-108836 19960718; CN 1224413 A CN 1997-194561 19970307; JP 2000506525 W JP 1997-532461 19970307, WO 1997-NL114 19970307; EP 888274 B1 EP 1997-908575 19970307, WO 1997-NL114 19970307; DE 69703035 E DE 1997-603035 19970307, EP 1997-908575 19970307, WO 1997-NL114 19970307; KR 99087823 A WO 1997-NL114 19970307, KR 1998-707364 19980914; ES 2152085 T3

EP 1997-908575 19970307
FDT AU 9720451 A Based on WO 9733854; EP 888274 A1 Based on WO 9733854; JP 2000506525 W Based on WO 9733854; EP 888274 B1 Based on WO 9733854; DE 69703035 E Based on EP 888274, Based on WO 9733854; KR 99087823 A Based on WO 9733854; ES 2152085 T3 Based on EP 888274
PRAI US 1996-616721 19960315
AB WO 9733854 A UPAB: 20010207
Preparation of a terminal aldehyde by hydroformylation by reacting an ethylenically unsaturated organic compound with carbon monoxide and hydrogen in the presence of a **catalyst** system comprising iridium or rhodium and a bidentate organic phosphate ligand of formula (1): formula (1)

The **phosphorus** atoms of the phosphate ligand are joined by a 2,2'-dihydroxyl-1,1'-bi:naphthalene bridging group of formula (Q): formula (Q)

R1 and R2 = substituents other than hydrogen; R3 and R4 = substituted monovalent aryl groups and/or any one of OR3 and OR4 connected to one **phosphorus** atom forms an -O-R5-O- group; R5 = a divalent organic group containing 1-2 aryl groups.

USE - The process is useful, eg. for preparation of an alkyl 5-formylvalerate by hydroformylation of an alkyl 3-pentenoate (claimed) and give moderately high selectivities in the preparation of 5-formyl-valero-nitrile (which is a precursor of caprolactam) from 3-pentenenitrile (claimed).

ADVANTAGE - The **catalyst** has high performance (selectivity and/or activity), providing high selectivities (eg. > 98% linear products) and high conversions (eg. > 73%) to terminal aldehyde compounds and can be used for a prolonged period of time. The advantages are particularly pronounced when using internally unsaturated organic compounds, compared with prior art hydroformylation processes which gave lower selectivity to terminal aldehydes, more hydrogenation of the olefinic double bond and/or lower catalytic activity. The process can be carried out continuously. The linearity (linear aldehydes/(linear + branched aldehydes)) is high, which facilitates the isolation of the desired terminal aldehyde from a mixture of terminal and branched aldehydes. Preparation of an alkyl 5-formylvalerate by hydroformylation of an alkyl 3-pentenoate can be carried out in the presence of alkyl 2-pentenoate without loss of **catalyst** activity.
Dwg.0/0

L14 ANSWER 5 OF 5 WPIDS (C) 2003 THOMSON DERWENT
AN 1989-349683 [48] WPIDS
DNC C1989-154947
TI **Catalysed** 3-pentenoate ester(s) isomerisation - by contacting with **catalyst** of zero valent nickel complex with acid promoter.
DC E17 J04
IN BURKE, P M; HERRON, N; MCLAIN, S J
PA (DUPO) DU PONT DE NEMOURS & CO E I
CYC 10
PI EP 343598 A 19891129 (198948)* EN 8p
R: BE DE FR GB IT LU NL
JP 02025450 A 19900126 (199010)
US 4895976 A 19900123 (199011) 5p
EP 343598 B1 19930707 (199327) EN 8p
R: BE DE FR GB IT LU NL
DE 68907443 E 19930812 (199333)
CA 1324612 C 19931123 (199402)
ADT EP 343598 A EP 1989-109252 19890523; JP 02025450 A JP 1989-127980

19890523; US 4895976 A US 1988-197221 19880523; EP 343598 B1 EP 1989-109252 19890523; DE 68907443 E DE 1989-607443 19890523, EP 1989-109252 19890523; CA 1324612 C CA 1989-600284 19890519

FDT DE 68907443 E Based on EP 343598

PRAI US 1988-197221 19880523

AB EP 343598 A UPAB: 19930923

3-pentenoate esters, of formula CH3-CH=CH-CH2-CO2R (where R = 1-8C alkyl) (I), are isomerised to 4-pentenoate esters, of formula CH2=CH-CH2-CH2-CO2R (II), in a new process. (I) are contacted with a **catalyst** of zero valent nickel complex with an acid promoter, at temps. 80-200 deg C for up to 1 hr. at pressures 15-200 psig.

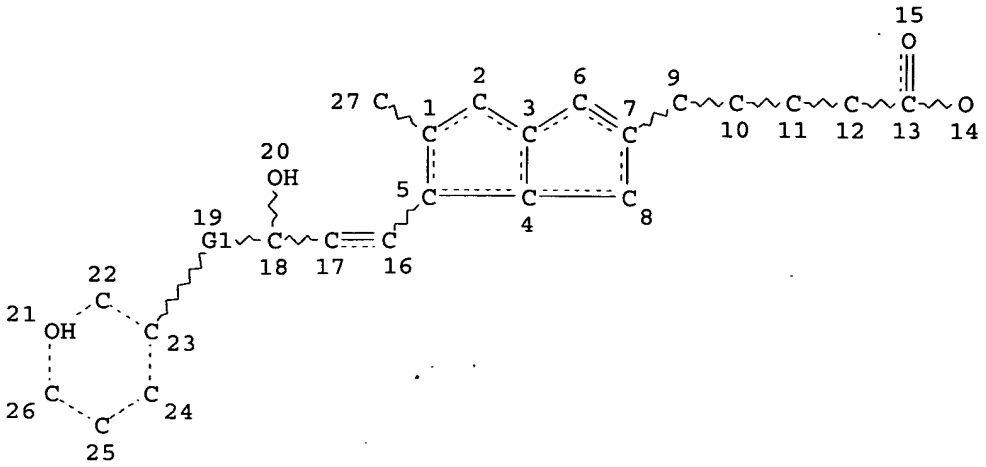
Pref. Ni **catalyst** is a nickel hydride complex of formula HNi(PYZ)n+ X- where P = **phosphorous**, Z = one of R' and OR' where R' = 1-18C hydrocarbyl radicals that may be substd. with -Cl, -O- or CN, and Y = two Zs and -R"- or -O-R"-O- where R" = 2-12C hydrocarbylene, n = integer 3 or 4 and X- = anion of a strong heterogeneous or homogeneous acid. (I) is **methyl**-3-**pentenoate**. The anion X- is acid exchanged y-zeolites or acidic amorphous silica-aluminates, or the acids sulphuric, fluorosulphonic, hexafluorosulphonic, methylsulphonic, trifluoromethylsulphonic and trifluoroacetic.

ADVANTAGE - The Ni **catalysts** are relative cheap, high active and selective for isomerisation of (I) to (II).

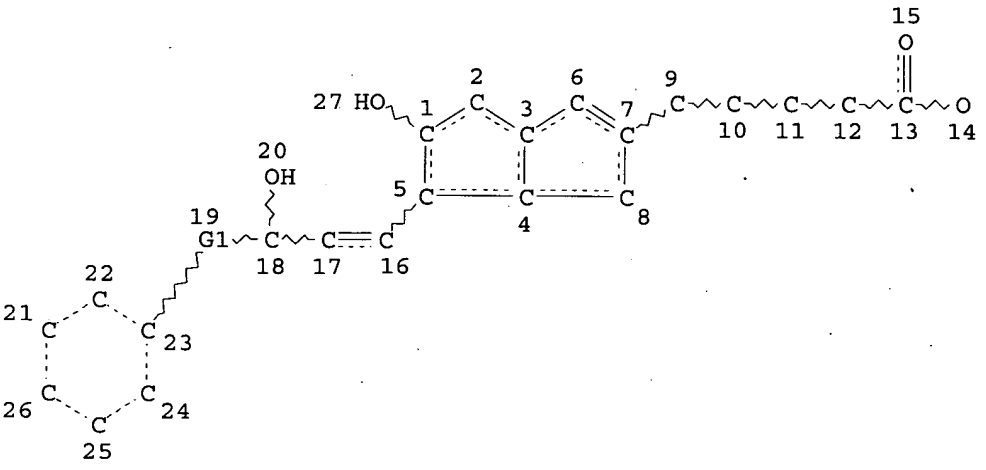
0/0

08/05
1999

ENTER (DIS), GRA, NOD, BON OR ?:nod 21 oh, rep g1=(1-10)ch2, dis



REP G1=(1-10) CH2
ENTER (DIS), GRA, NOD, BON OR ?:nod 21 c, nod 27 oh, dis



REP G1=(1-10) CH2
ENTER (DIS), GRA, NOD, BON OR ?:end
L1 STRUCTURE CREATED

=> save temp l1
ENTER NAME OR (END):sn10048964/q
QUERY L1 HAS BEEN SAVED AS 'SN10048964/Q'

=> search l1 sss full
FULL SEARCH INITIATED 11:08:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 15281 TO ITERATE

100.0% PROCESSED 15281 ITERATIONS 78 ANSWERS
SEARCH TIME: 00.00.01

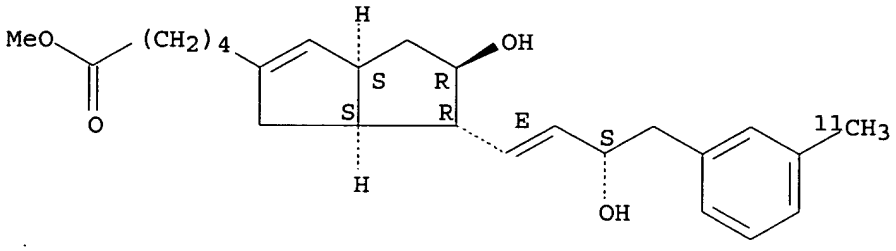
L2 78 SEA SSS FUL L1

=> dis l2 1- sub bib abs
YOU HAVE REQUESTED DATA FROM 78 ANSWERS - CONTINUE? Y/(N):y

L2 ANSWER 1 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 312693-38-2 REGISTRY
CN 2-Pentalenepentanoic acid, 3,3a,4,5,6,6a-hexahydro-5-hydroxy-4-[(1E,3S)-3-hydroxy-4-[3-(methyl-11C)phenyl]-1-butenyl]-, methyl ester, (3aS,4R,5R,6aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H34 O4

SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



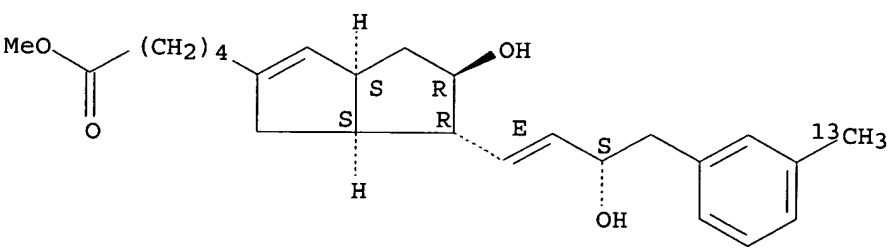
1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

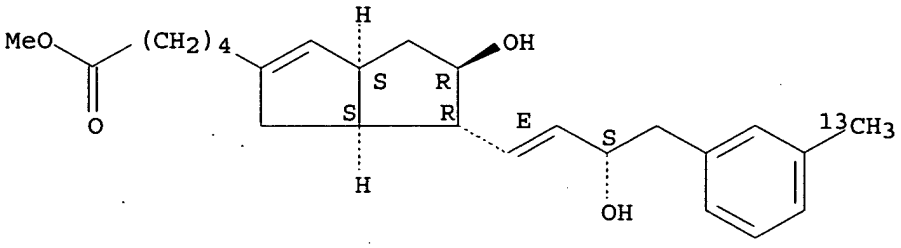
REFERENCE 1

AN 134:41988 CA
TI Rapid Methylation for the Synthesis of a 11C-Labeled Tolylisocarbacyclin Imaging the IP2 Receptor in a Living Human Brain
AU Suzuki, M.; Doi, H.; Kato, K.; Bjorkman, M.; Langstrom, B.; Watanabe, Y.; Noyori, R.
CS Faculty of Engineering, Department of Biomolecular Science, Gifu University, Gifu, 501-1193, Japan
SO Tetrahedron (2000), 56(42), 8263-8273
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier Science Ltd.
DT Journal
LA English
AB A rapid method for Pd-promoted cross-coupling of Me iodide and tributyltin derivs. of tolylisocarbacyclins was developed with the objective of applying to the PET study on the IP2 receptor in a living human brain. The high efficiency is obtainable for both of the one-pot operation using a large excess of CuCl and the stepwise operation consisting of the initial prepn. of a methylpalladium complex followed by mixing with the remaining requisite materials for the cross-coupling. The latter protocol allowed for the highly reproducible synthesis of an actual PET tracer with total radioactivity of several GBq. Several stannanes could be employed as precursors of PET tracers in this rapid cross-coupling reaction.
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 2 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 312693-36-0 REGISTRY
CN 2-Pentalenepentanoic acid, 3,3a,4,5,6,6a-hexahydro-5-hydroxy-4-[(1E,3S)-3-hydroxy-4-[3-(methyl-13C)phenyl]-1-butenyl]-, methyl ester, (3aS,4R,5R,6aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25•H34 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.





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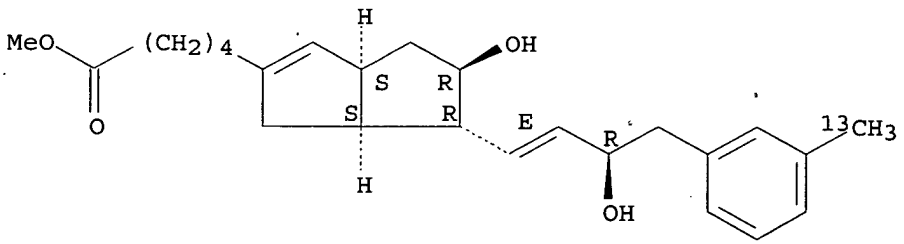
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 3 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 312693-35-9 REGISTRY
CN 2-Pentalenepentanoic acid, 3,3a,4,5,6,6a-hexahydro-5-hydroxy-4-[(1E,3R)-3-hydroxy-4-[3-(methyl-13C)phenyl]-1-butenyl]-, methyl ester, (3aS,4R,5R,6aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H34 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



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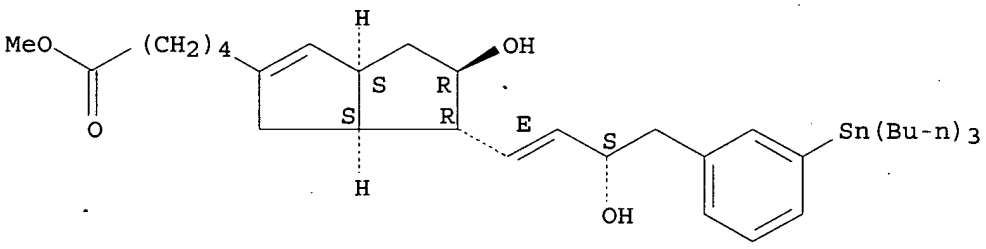
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 4 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 312693-26-8 REGISTRY
CN 2-Pentalenepentanoic acid, 3,3a,4,5,6,6a-hexahydro-5-hydroxy-4-[(1E,3S)-3-hydroxy-4-[3-(tributylstannyl)phenyl]-1-butenyl]-, methyl ester, (3aS,4R,5R,6aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C36 H58 O4 Sn
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 134:41988 CA
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CS Faculty of Engineering, Department of Biomolecular Science, Gifu University, Gifu, 501-1193, Japan
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PB Elsevier Science Ltd.
DT Journal

LA English
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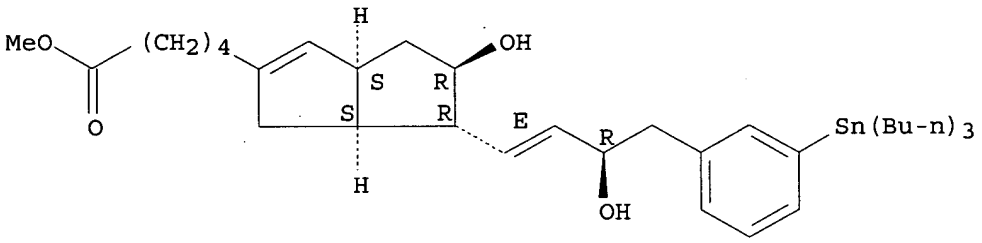
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 5 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 312693-25-7 REGISTRY
CN 2-Pentalenepentanoic acid, 3,3a,4,5,6,6a-hexahydro-5-hydroxy-4-[(1E,3R)-3-hydroxy-4-[3-(tributylstannyl)phenyl]-1-butenyl]-, methyl ester, (3aS,4R,5R,6aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C36 H58 O4 Sn
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.
Double bond geometry as shown.



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1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

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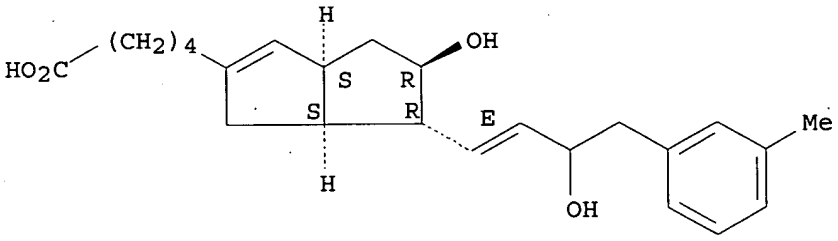
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 6 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 235091-54-0 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E)-3-hydroxy-4-(3-methylphenyl)-1-butenyl]-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H32 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

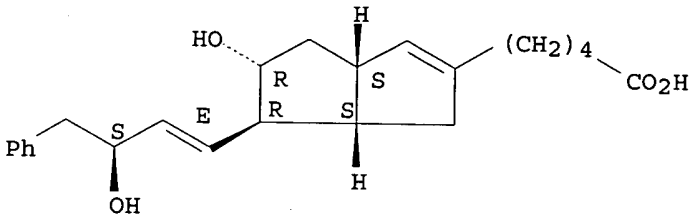
REFERENCE 1

AN 131:139854 CA
TI A novel subtype of prostacyclin receptor in the central nervous system
AU Watanabe, Yumiko; Matsumura, Kiyoshi; Takechi, Hajime; Kato, Koichi; Morii, Hiroshi; Bjorkman, Margareta; Langstrom, Bengt; Noyori, Ryoji; Suzuki, Masaaki; Watanabe, Yasuyoshi
CS Subfemtomole Biorecognition Project, ICORP, Department of Neuroscience, Osaka Bioscience Institute, Japan Science and Technology Corporation, Osaka, 565-0874, Japan
SO Journal of Neurochemistry (1999), 72(6), 2583-2592
CODEN: JONRA9; ISSN: 0022-3042
PB Lippincott Williams & Wilkins
DT Journal
LA English
AB Recently, in the course of the authors' search for the prostacyclin receptor in the brain, the authors found a novel subtype, designated as IP2, which was finely discriminated by use of the specific ligand (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (15R-TIC) and specifically localized in the rostral part of the brain. In the present study, the tritiated compd. 15R-[15-3H]TIC was synthesized and utilized for more specific research on IP2. The specificity of binding to rat brain regions was confirmed by use of several prostacyclin derivs. including 15S-TIC. Mapping of 15R- and 15S-[3H]TIC binding in adjacent pairs of frozen sections of rat brain demonstrated a quite similar pattern of distribution in almost all rostral brain regions, indicating that the regions may contain only the IP2 subtype. 15R-[3H]TIC binding was very faint as compared with 15S-[3H]TIC binding in the caudal medullary region. High densities of 15R-[3H]TIC binding sites were shown in the dorsal part of the lateral septal nucleus, thalamic nuclei, limbic structures, and some of the cortical regions. Scatchard plot anal. showed two components of high-affinity 15R-[3H]TIC binding in the rostral regions, one with a KD value at .apprx.1 nM and the other with .apprx.30 nM. These results strengthen the authors' previous finding that a different subtype of prostacyclin receptor is expressed in the CNS, and the map with 15R-[3H]TIC obtained here could guide further studies on the mol. and functional properties of the IP2.

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 7 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 235091-53-9 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E,3S)-3-hydroxy-4-phenyl-1-butenyl]-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H30 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

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CS Subfemtomole Biorecognition Project, ICORP, Department of Neuroscience, Osaka Bioscience Institute, Japan Science and Technology Corporation, Osaka, 565-0874, Japan
SO Journal of Neurochemistry (1999), 72(6), 2583-2592
CODEN: JONRA9; ISSN: 0022-3042
PB Lippincott Williams & Wilkins
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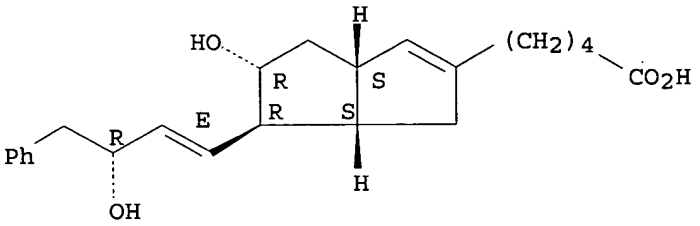
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 8 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 235091-51-7 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E,3R)-3-hydroxy-4-phenyl-1-butenyl]-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H30 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



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CS Subfemtomole Biorecognition Project, ICORP, Department of Neuroscience, Osaka Bioscience Institute, Japan Science and Technology Corporation, Osaka, 565-0874, Japan
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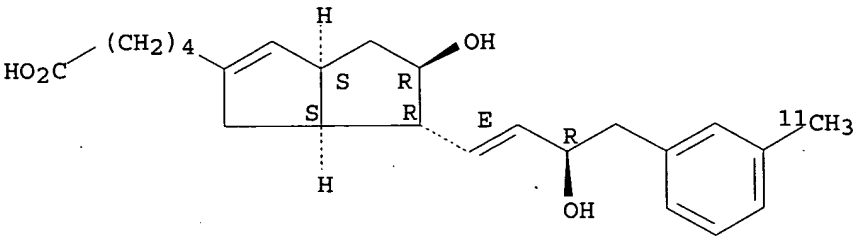
LA English
AB Recently, in the course of the authors' search for the prostacyclin receptor in the brain, the authors found a novel subtype, designated as IP2, which was finely discriminated by use of the specific ligand (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (15R-TIC) and specifically localized in the rostral part of the brain. In the present study, the tritiated compd. 15R-[15-3H]TIC was synthesized and utilized for more specific research on IP2. The specificity of binding to rat brain regions was confirmed by use of several prostacyclin derivs. including 15S-TIC. Mapping of 15R- and 15S-[3H]TIC binding in adjacent pairs of frozen sections of rat brain demonstrated a quite similar pattern of distribution in almost all rostral brain regions, indicating that the regions may contain only the IP2 subtype. 15R-[3H]TIC binding was very faint as compared with 15S-[3H]TIC binding in the caudal medullary region. High densities of 15R-[3H]TIC binding sites were shown in the dorsal part of the lateral septal nucleus, thalamic nuclei, limbic structures, and some of the cortical regions. Scatchard plot anal. showed two components of high-affinity 15R-[3H]TIC binding in the rostral regions, one with a KD value at .apprx.1 nM and the other with .apprx.30 nM. These results strengthen the authors' previous finding that a different subtype of prostacyclin receptor is expressed in the CNS, and the map with 15R-[3H]TIC obtained here could guide further studies on the mol. and functional properties of the IP2.
RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 9 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 223778-94-7 REGISTRY
CN 2-Pentalenepentanoic acid, 3,3a,4,5,6,6a-hexahydro-5-hydroxy-4-[(1E,3R)-3-hydroxy-4-[3-(methyl-11C)phenyl]-1-butenyl]-, (3aS,4R,5R,6aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H32 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



2 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:129774 CA
TI Design of prostaglandins with high binding affinity and selectivity for an IP2 receptor in the central nervous system and their biological activity
AU Suzuki, Masaaki; Kato, Koichi; Noyori, Ryoji; Watanabe, Yumiko; Sato, Takumi; Matsumura, Kiyoshi; Watanabe, Yasuyoshi
CS Faculty of Engineering, Gifu University, Japan
SO Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1998), 40th, 145-150
CODEN: TYKYDS
PB Nippon Kagakkai
DT Journal
LA Japanese
GI

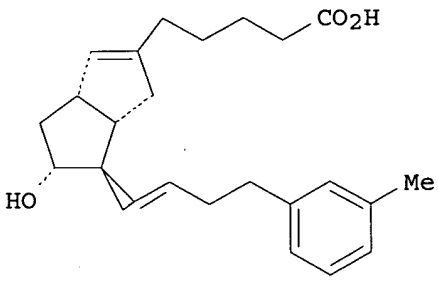
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The role of prostacyclin (PGI2) in the central nervous system (CNS) has still been unclear because of the lack of a specific ligand for a PGI2 receptor in CNS. In this context, the authors recently elaborated 15R-TIC (I; R = OH, R1 = H) with high binding affinity and selectivity for novel IP2 receptor which is specifically expressed in CNS neurons. The R configuration of the hydroxy-bearing C(15) in 15R-TIC is fascinating, because, in general, the configuration of biol. active PGs at C(15) position is known to be S. In this symposium, the authors describe synthesis of the TIC derivs. for structure-binding affinity relationship in addn. to biol. actions. 15-Deoxy-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (I; R = R1 = H) (referred to as 15-deoxy-TIC) exhibited, among others, highest binding affinity and selectivity for a IP2 receptor. I (R = R1 = H) has been prepd. based on the combination of the Witting reaction and Pd(0)-mediated coupling of an allyl carbonate and a sulfone. Thus, Witting reaction of aldehyde II (R2 = CHO, R3 = THP) and a Ph3P:CHCHO led to II [R2 = (E)-CH:CHCHO, R3 = THP]. The redn. of this followed by methoxycarbonylation gave allyl carbonate II [R2 = (E)-CH:CHCH2-OCO2Me, R3 = THP] which was treated with disulfone III in the presence of a 1:1 mixt. of Pd(0) and diphenylphosphinoethane to give II [R2 = (E)-CH:CHCH2-C(SO2Ph)2C6H4Me-m, R3 = THP]. Reductive removal of Ph

sulfonyl groups of this and subsequent deprotection gave II (R2 = CH2CH2C6H4Me-m, R3 = H), which was hydrolyzed to give I (R = R1 = H). I (R, R1 = OH, H; H, H) prevented apoptotic cell death of hippocampal neurons induced under high oxygen (50%) atm., whereas I (R = H, R1 = OH), isocarbacyclin, and natural PGs except for PGI2 did not show such a biol. effect.

REFERENCE 2

AN 130:325022 CA
TI 15-Deoxy-16-(m-tolyl)-17,18,19,20-tetranorisocarbacyclin: a simple TIC derivative with potent anti-apoptotic activity for neuronal cells
AU Suzuki, Masaaki; Kato, Koichi; Noyori, Ryoji; Watanabe, Yumiko; Satoh, Takumi; Matsumura, Kiyoshi; Watanabe, Yasuyoshi
CS Faculty of Engineering, Department of Biomolecular Science, Gifu University, Gifu, 501-1193, Japan
SO Chemical Communications (Cambridge) (1999), (4), 307-308
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
GI

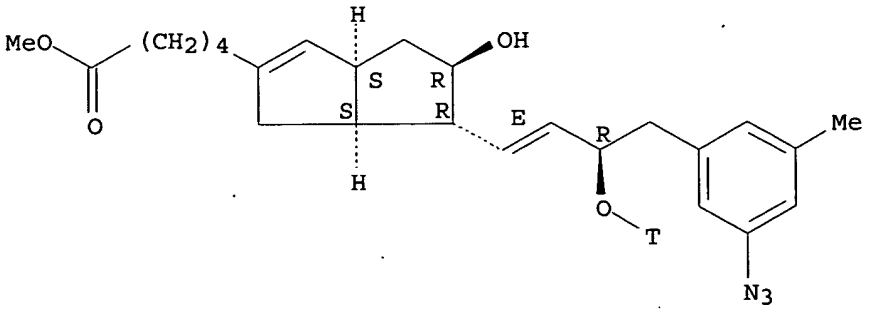


I

AB Biol. remarkable 15-deoxy-TIC (I) has been realized by the removal of the C(15) chiral center in 15R-TIC, a stable ligand for a CNS-type prostacyclin receptor (IP2); this deoxy deriv. exhibits ten-fold higher affinity and selectivity than 15R-TIC for the IP2 receptor in correlation with the anti-apoptotic activity for neuronal cells.
RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 10 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 207284-07-9 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[(1E,3R)-4-(3-azido-5-methylphenyl)-3-(hydroxy-t)-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 6-[4-(3-azido-5-methylphenyl)-3-(hydroxy-t)-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]-
FS STEREOSEARCH
MF C25 H32 N3 O4 T
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 129:4520 CA
TI Preparation of isocarbacyclin derivatives, their radiolabeled compounds, and their use as photoaffinity labeling probes
IN Watanabe, Yasuyoshi; Hasato, Atsuo; Watanabe, Yumiko; Suzuki, Masaki
PA Foundation for Scientific Technology Promotion, Japan; Hasato, Atsuo
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10087608	A2	19980407	JP 1996-243122	19960913

PRAI JP 1996-243122 19960913
GI

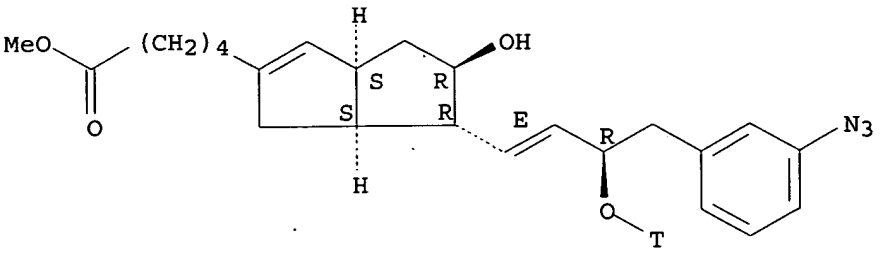
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The derivs. I (R1 = H, alkyl, cation; R2 = alkylene; R3 = H, Me) are prepd. by treatment of Horner-Emmons reagents II with formyl compds. III (R4 = C1-5 alkyl; R5 = H, tetrahydropyranyl) in the presence of bases, deprotection of OH-protective group if necessary, redn. of the resulting ketones IV, and hydrolysis if necessary. Also claimed are I labeled with 3H, 11C, or 14C at the arbitrary position and photoaffinity labeling using the radiolabeled I as probes, esp. for labeling of prostacyclin receptors. I are also useful as drugs for central nervous system disorders. A MeOH soln. of 16-(3-azidophenyl)-15-dehydro-17,18,19,20-tetranorisocarbacyclin Me ester prepd. from di-Me 2-oxo-3-(3-azidophenyl)propylphosphonate and III (R4 = Me, R5 = H), was treated with CeCl3.7H2O at room temp. then NaBH4 at 0.degree., and the resulting product was fractionated by silica gel chromatog. to give 48% 16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester and 49% 15-epi-16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester (V). A MeOH soln. of V was treated with an aq. NaOH soln. to give 96% free acid (VI). VI dose-dependently displaced [3H]-15S-(16-m-tolyl)isocarbacyclin on a rat brain slice.

L2 ANSWER 11 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 207284-06-8 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[(1E,3R)-4-(3-azidophenyl)-3-(hydroxy-t)-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 6-[4-(3-azidophenyl)-3-(hydroxy-t)-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]-
FS STEREOSEARCH
MF C24 H30 N3 O4 T

SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 129:4520 CA
TI Preparation of isocarbacyclin derivatives, their radiolabeled compounds, and their use as photoaffinity labeling probes
IN Watanabe, Yasuyoshi; Hasato, Atsuo; Watanabe, Yumiko; Suzuki, Masaki
PA Foundation for Scientific Technology Promotion, Japan; Hasato, Atsuo
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10087608	A2	19980407	JP 1996-243122	19960913
PRAI	JP 1996-243122		19960913		

GI

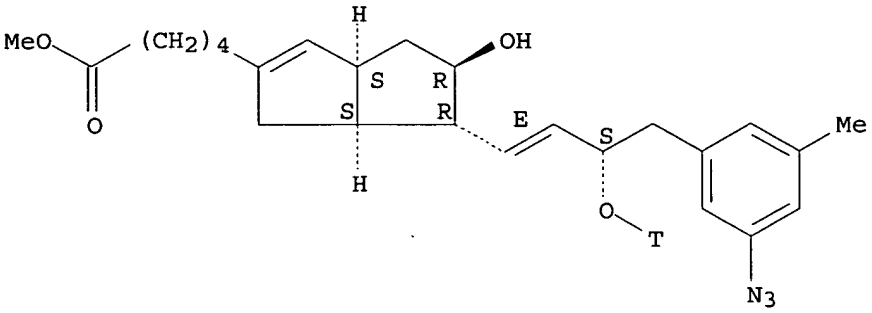
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The derivs. I (R1 = H, alkyl, cation; R2 = alkylene; R3 = H, Me) are prepd. by treatment of Horner-Emmons reagents II with formyl compds. III (R4 = C1-5 alkyl; R5 = H, tetrahydropyranyl) in the presence of bases, deprotection of OH-protective group if necessary, redn. of the resulting ketones IV, and hydrolysis if necessary. Also claimed are I labeled with 3H, 11C, or 14C at the arbitrary position and photoaffinity labeling using the radiolabeled I as probes, esp. for labeling of prostacyclin receptors. I are also useful as drugs for central nervous system disorders. A MeOH soln. of 16-(3-azidophenyl)-15-dehydro-17,18,19,20-tetranorisocarbacyclin Me ester prepd. from di-Me 2-oxo-3-(3-azidophenyl)propylphosphonate and III (R4 = Me, R5 = H), was treated with CeCl3.7H2O at room temp. then NaBH4 at 0.degree., and the resulting product was fractionated by silica gel chromatog. to give 48% 16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester and 49% 15-epi-16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester (V). A MeOH soln. of V was treated with an aq. NaOH soln. to give 96% free acid (VI). VI dose-dependently displaced [3H]-15S-(16-m-tolyl)isocarbacyclin on a rat brain slice.

L2 ANSWER 12 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 207284-04-6 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[(1E,3S)-4-(3-azido-5-methylphenyl)-3-(hydroxy-t)-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 6-[4-(3-azido-5-methylphenyl)-3-(hydroxy-t)-1-

butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]-
FS STEREOSEARCH
MF C25 H32 N3 O4 T
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 129:4520 CA
TI Preparation of isocarbacyclin derivatives, their radiolabeled compounds, and their use as photoaffinity labeling probes
IN Watanabe, Yasuyoshi; Hasato, Atsuo; Watanabe, Yumiko; Suzuki, Masaki
PA Foundation for Scientific Technology Promotion, Japan; Hasato, Atsuo
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10087608	A2	19980407	JP 1996-243122	19960913
PRAI	JP 1996-243122		19960913		

GI

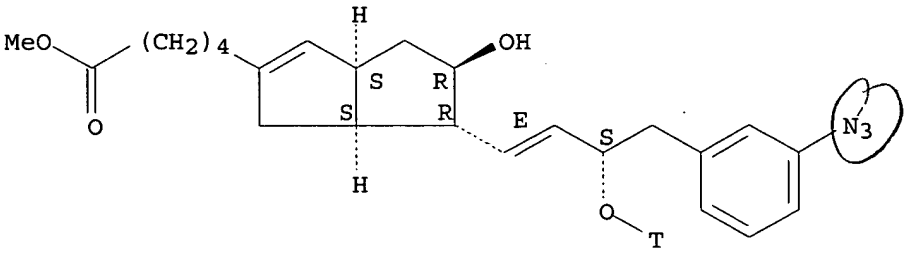
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The derivs. I (R1 = H, alkyl, cation; R2 = alkylene; R3 = H, Me) are prepd. by treatment of Horner-Emmons reagents II with formyl compds. III (R4 = C1-5 alkyl; R5 = H, tetrahydropyranyl) in the presence of bases, deprotection of OH-protective group if necessary, redn. of the resulting ketones IV, and hydrolysis if necessary. Also claimed are I labeled with 3H, 11C, or 14C at the arbitrary position and photoaffinity labeling using the radiolabeled I as probes, esp. for labeling of prostacyclin receptors. I are also useful as drugs for central nervous system disorders. A MeOH soln. of 16-(3-azidophenyl)-15-dehydro-17,18,19,20-tetranorisocarbacyclin Me ester prepd. from di-Me 2-oxo-3-(3-azidophenyl)propylphosphonate and III (R4 = Me, R5 = H), was treated with CeCl3.7H2O at room temp. then NaBH4 at 0.degree., and the resulting product was fractionated by silica gel chromatog. to give 48% 16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester and 49% 15-epi-16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester (V). A MeOH soln. of V was treated with an aq. NaOH soln. to give 96% free acid (VI). VI dose-dependently displaced [3H]-15S-(16-m-tolyl)isocarbacyclin on a rat brain slice.

L2 ANSWER 13 OF 78 REGISTRY COPYRIGHT 2003 ACS

RN 207284-02-4 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[(1E,3S)-4-(3-azidophenyl)-3-(hydroxy-t)-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 6-[4-(3-azidophenyl)-3-(hydroxy-t)-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]-
FS STEREOSEARCH
MF C24 H30 N3 O4 T
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 129:4520 CA
TI Preparation of isocarbacyclin derivatives, their radiolabeled compounds, and their use as photoaffinity labeling probes
IN Watanabe, Yasuyoshi; Hasato, Atsuo; Watanabe, Yumiko; Suzuki, Masaki
PA Foundation for Scientific Technology Promotion, Japan; Hasato, Atsuo
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10087608	A2	19980407	JP 1996-243122	19960913
PRAI	JP 1996-243122		19960913		

GI

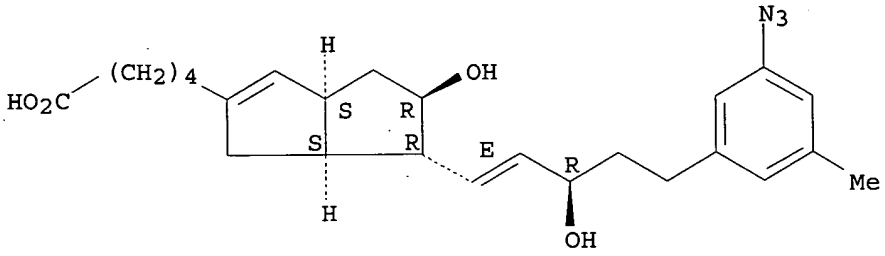
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The derivs. I (R1 = H, alkyl, cation; R2 = alkylene; R3 = H, Me) are prepd. by treatment of Horner-Emmons reagents II with formyl compds. III (R4 = C1-5 alkyl; R5 = H, tetrahydropyranyl) in the presence of bases, deprotection of OH-protective group if necessary, redn. of the resulting ketones IV, and hydrolysis if necessary. Also claimed are I labeled with 3H, 11C, or 14C at the arbitrary position and photoaffinity labeling using the radiolabeled I as probes, esp. for labeling of prostacyclin receptors. I are also useful as drugs for central nervous system disorders. A MeOH soln. of 16-(3-azidophenyl)-15-dehydro-17,18,19,20-tetranorisocarbacyclin Me ester prepd. from di-Me 2-oxo-3-(3-azidophenyl)propylphosphonate and III (R4 = Me, R5 = H), was treated with CeCl3.7H2O at room temp. then NaBH4 at 0.degree., and the resulting product was fractionated by silica gel chromatog. to give 48% 16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester and 49% 15-epi-16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester (V). A MeOH soln. of V was treated with an aq. NaOH soln. to give 96% free acid (VI). VI

dose-dependently displaced [3H]-15S-(16-m-tolyl)isocarbacyclin on a rat brain slice.

L2 ANSWER 14 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 207283-99-6 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[(1E,3R)-5-(3-azido-5-methylphenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 6-[5-(3-azido-5-methylphenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]-
FS STEREOSEARCH
MF C25 H33 N3 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 129:4520 CA
TI Preparation of isocarbacyclin derivatives, their radiolabeled compounds, and their use as photoaffinity labeling probes
IN Watanabe, Yasuyoshi; Hasato, Atsuo; Watanabe, Yumiko; Suzuki, Masaki
PA Foundation for Scientific Technology Promotion, Japan; Hasato, Atsuo
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10087608	A2	19980407	JP 1996-243122	19960913
PRAI	JP 1996-243122		19960913		

GI

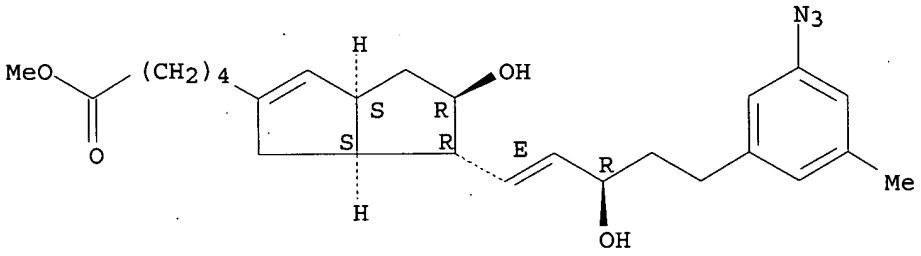
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The derivs. I (R1 = H, alkyl, cation; R2 = alkylene; R3 = H, Me) are prepd. by treatment of Horner-Emmons reagents II with formyl compds. III (R4 = C1-5 alkyl; R5 = H, tetrahydropyranyl) in the presence of bases, deprotection of OH-protective group if necessary, redn. of the resulting ketones IV, and hydrolysis if necessary. Also claimed are I labeled with 3H, 11C, or 14C at the arbitrary position and photoaffinity labeling using the radiolabeled I as probes, esp. for labeling of prostacyclin receptors. I are also useful as drugs for central nervous system disorders. A MeOH soln. of 16-(3-azidophenyl)-15-dehydro-17,18,19,20-tetranorisocarbacyclin Me ester prepd. from di-Me 2-oxo-3-(3-azidophenyl)propylphosphonate and III (R4 = Me, R5 = H), was treated with CeCl3.7H2O at room temp. then NaBH4 at 0.degree., and the resulting product was fractionated by silica

gel chromatog. to give 48% 16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester and 49% 15-epi-16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester (V). A MeOH soln. of V was treated with an aq. NaOH soln. to give 96% free acid (VI). VI dose-dependently displaced [3H]-15S-(16-m-tolyl)isocarbacyclin on a rat brain slice.

L2 ANSWER 15 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 207283-97-4 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[(1E,3R)-5-(3-azido-5-methylphenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 6-[5-(3-azido-5-methylphenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]-
FS STEREOSEARCH
MF C26 H35 N3 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 129:4520 CA
TI Preparation of isocarbacyclin derivatives, their radiolabeled compounds, and their use as photoaffinity labeling probes
IN Watanabe, Yasuyoshi; Hasato, Atsuo; Watanabe, Yumiko; Suzuki, Masaki
PA Foundation for Scientific Technology Promotion, Japan; Hasato, Atsuo
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10087608	A2	19980407	JP 1996-243122	19960913
PRAI	JP 1996-243122		19960913		

GI

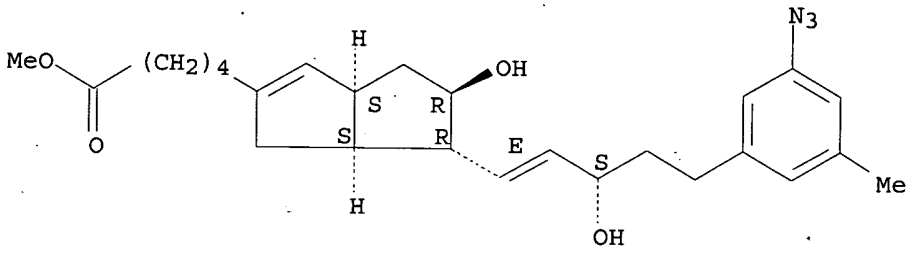
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The derivs. I (R1 = H, alkyl, cation; R2 = alkylene; R3 = H, Me) are prepd. by treatment of Horner-Emmons reagents II with formyl compds. III (R4 = C1-5 alkyl; R5 = H, tetrahydropyranyl) in the presence of bases, deprotection of OH-protective group if necessary, redn. of the resulting ketones IV, and hydrolysis if necessary. Also claimed are I labeled with 3H, 11C, or 14C at the arbitrary position and photoaffinity labeling using the radiolabeled I as probes, esp. for labeling of prostacyclin receptors. I are also useful as drugs for central nervous system disorders. A MeOH

soln. of 16-(3-azidophenyl)-15-dehydro-17,18,19,20-tetranorisocarbacyclin Me ester prepd. from di-Me 2-oxo-3-(3-azidophenyl)propylphosphonate and III (R4 = Me, R5 = H), was treated with CeCl3.7H2O at room temp. then NaBH4 at 0.degree., and the resulting product was fractionated by silica gel chromatog. to give 48% 16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester and 49% 15-epi-16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester (V). A MeOH soln. of V was treated with an aq. NaOH soln. to give 96% free acid (VI). VI dose-dependently displaced [3H]-15S-(16-m-tolyl)isocarbacyclin on a rat brain slice.

L2 ANSWER 16 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 207283-94-1 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[(1E,3S)-5-(3-azido-5-methylphenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 6-[5-(3-azido-5-methylphenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]-
FS STEREOSEARCH
MF C26 H35 N3 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 129:4520 CA
TI Preparation of isocarbacyclin derivatives, their radiolabeled compounds, and their use as photoaffinity labeling probes
IN Watanabe, Yasuyoshi; Hasato, Atsuo; Watanabe, Yumiko; Suzuki, Masaki
PA Foundation for Scientific Technology Promotion, Japan; Hasato, Atsuo
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10087608	A2	19980407	JP 1996-243122	19960913
PRAI	JP 1996-243122		19960913		

GI

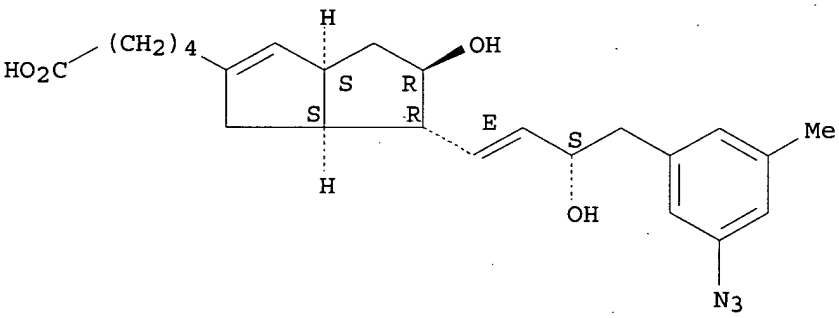
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The derivs. I (R1 = H, alkyl, cation; R2 = alkylene; R3 = H, Me) are prepd. by treatment of Horner-Emmons reagents II with formyl compds. III (R4 = C1-5 alkyl; R5 = H, tetrahydropyranyl) in the presence of bases, deprotection of OH-protective group if necessary, redn. of the resulting

ketones IV, and hydrolysis if necessary. Also claimed are I labeled with 3H, 11C, or 14C at the arbitrary position and photoaffinity labeling using the radiolabeled I as probes, esp. for labeling of prostacyclin receptors. I are also useful as drugs for central nervous system disorders. A MeOH soln. of 16-(3-azidophenyl)-15-dehydro-17,18,19,20-tetranorisocarbacyclin Me ester prepd. from di-Me 2-oxo-3-(3-azidophenyl)propylphosphonate and III (R4 = Me, R5 = H), was treated with CeCl3.7H2O at room temp. then NaBH4 at 0.degree., and the resulting product was fractionated by silica gel chromatog. to give 48% 16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester and 49% 15-epi-16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester (V). A MeOH soln. of V was treated with an aq. NaOH soln. to give 96% free acid (VI). VI dose-dependently displaced [3H]-15S-(16-m-tolyl)isocarbacyclin on a rat brain slice.

L2 ANSWER 17 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 207283-75-8 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[(1E,3S)-4-(3-azido-5-methylphenyl)-3-hydroxy-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 6-[4-(3-azido-5-methylphenyl)-3-hydroxy-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]-
FS STEREOSEARCH
MF C24 H31 N3 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 129:4520 CA
TI Preparation of isocarbacyclin derivatives, their radiolabeled compounds, and their use as photoaffinity labeling probes
IN Watanabe, Yasuyoshi; Hasato, Atsuo; Watanabe, Yumiko; Suzuki, Masaki
PA Foundation for Scientific Technology Promotion, Japan; Hasato, Atsuo
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 10087608	A2	19980407	JP 1996-243122	19960913
PRAI JP 1996-243122		19960913		

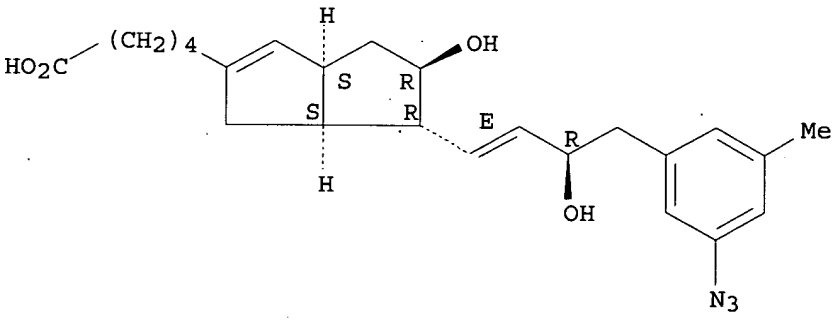
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The derivs. I (R1 = H, alkyl, cation; R2 = alkylene; R3 = H, Me) are prepd. by treatment of Horner-Emmons reagents II with formyl compds. III (R4 = C1-5 alkyl; R5 = H, tetrahydropyranyl) in the presence of bases, deprotection of OH-protective group if necessary, redn. of the resulting ketones IV, and hydrolysis if necessary. Also claimed are I labeled with 3H, 11C, or 14C at the arbitrary position and photoaffinity labeling using the radiolabeled I as probes, esp. for labeling of prostacyclin receptors. I are also useful as drugs for central nervous system disorders. A MeOH soln. of 16-(3-azidophenyl)-15-dehydro-17,18,19,20-tetranorisocarbacyclin Me ester prepd. from di-Me 2-oxo-3-(3-azidophenyl)propylphosphonate and III (R4 = Me, R5 = H), was treated with CeCl3.7H2O at room temp. then NaBH4 at 0.degree., and the resulting product was fractionated by silica gel chromatog. to give 48% 16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester and 49% 15-epi-16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester (V). A MeOH soln. of V was treated with an aq. NaOH soln. to give 96% free acid (VI). VI dose-dependently displaced [3H]-15S-(16-m-tolyl)isocarbacyclin on a rat brain slice.

L2 ANSWER 18 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 207283-71-4 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[(1E,3R)-4-(3-azido-5-methylphenyl)-3-hydroxy-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 6-[4-(3-azido-5-methylphenyl)-3-hydroxy-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]-
FS STEREOSEARCH
MF C24 H31 N3 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 129:4520 CA
TI Preparation of isocarbacyclin derivatives, their radiolabeled compounds, and their use as photoaffinity labeling probes
IN Watanabe, Yasuyoshi; Hasato, Atsuo; Watanabe, Yumiko; Suzuki, Masaki
PA Foundation for Scientific Technology Promotion, Japan; Hasato, Atsuo
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10087608	A2	19980407	JP 1996-243122	19960913

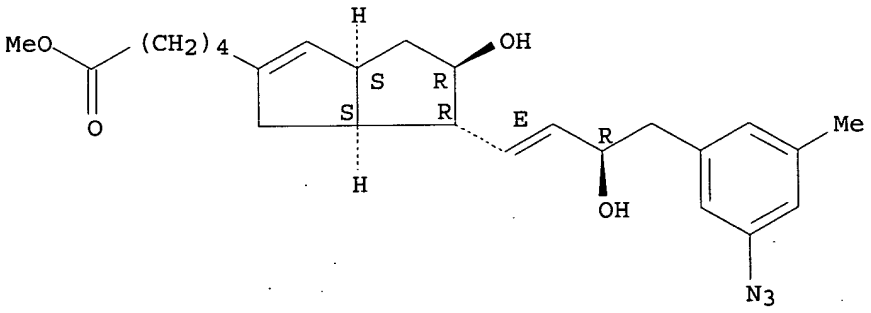
PRAI JP 1996-243122 19960913
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The derivs. I (R1 = H, alkyl, cation; R2 = alkylene; R3 = H, Me) are prepd. by treatment of Horner-Emmons reagents II with formyl compds. III (R4 = C1-5 alkyl; R5 = H, tetrahydropyranyl) in the presence of bases, deprotection of OH-protective group if necessary, redn. of the resulting ketones IV, and hydrolysis if necessary. Also claimed are I labeled with 3H, 11C, or 14C at the arbitrary position and photoaffinity labeling using the radiolabeled I as probes, esp. for labeling of prostacyclin receptors. I are also useful as drugs for central nervous system disorders. A MeOH soln. of 16-(3-azidophenyl)-15-dehydro-17,18,19,20-tetranorisocarbacyclin Me ester prepd. from di-Me 2-oxo-3-(3-azidophenyl)propylphosphonate and III (R4 = Me, R5 = H), was treated with CeCl3.7H2O at room temp. then NaBH4 at 0.degree., and the resulting product was fractionated by silica gel chromatog. to give 48% 16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester and 49% 15-epi-16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester (V). A MeOH soln. of V was treated with an aq. NaOH soln. to give 96% free acid (VI). VI dose-dependently displaced [3H]-15S-(16-m-tolyl)isocarbacyclin on a rat brain slice.

L2 ANSWER 19 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 207283-67-8 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[(1E,3R)-4-(3-azido-5-methylphenyl)-3-hydroxy-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 6-[4-(3-azido-5-methylphenyl)-3-hydroxy-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]-
FS STEREOSEARCH
MF C25 H33 N3 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 129:4520 CA
TI Preparation of isocarbacyclin derivatives, their radiolabeled compounds, and their use as photoaffinity labeling probes
IN Watanabe, Yasuyoshi; Hasato, Atsuo; Watanabe, Yumiko; Suzuki, Masaki
PA Foundation for Scientific Technology Promotion, Japan; Hasato, Atsuo
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF

DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10087608	A2	19980407	JP 1996-243122	19960913
PRAI	JP 1996-243122		19960913		

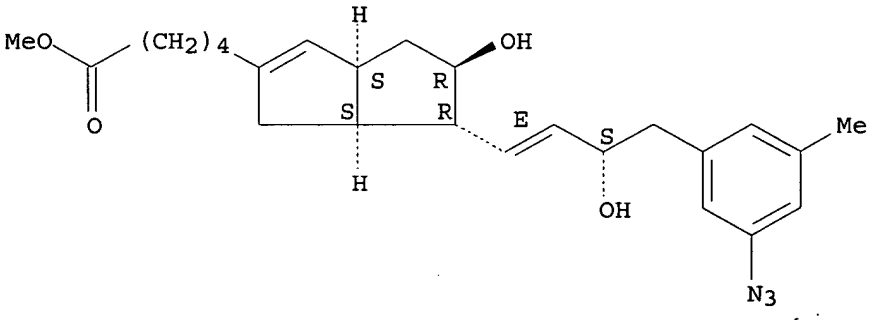
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The derivs. I (R1 = H, alkyl, cation; R2 = alkylene; R3 = H, Me) are prepd. by treatment of Horner-Emmons reagents II with formyl compds. III (R4 = C1-5 alkyl; R5 = H, tetrahydropyranyl) in the presence of bases, deprotection of OH-protective group if necessary, redn. of the resulting ketones IV, and hydrolysis if necessary. Also claimed are I labeled with 3H, 11C, or 14C at the arbitrary position and photoaffinity labeling using the radiolabeled I as probes, esp. for labeling of prostacyclin receptors. I are also useful as drugs for central nervous system disorders. A MeOH soln. of 16-(3-azidophenyl)-15-dehydro-17,18,19,20-tetranorisocarbacyclin Me ester prepd. from di-Me 2-oxo-3-(3-azidophenyl)propylphosphonate and III (R4 = Me, R5 = H), was treated with CeCl3.7H2O at room temp. then NaBH4 at 0.degree., and the resulting product was fractionated by silica gel chromatog. to give 48% 16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester and 49% 15-epi-16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester (V). A MeOH soln. of V was treated with an aq. NaOH soln. to give 96% free acid (VI). VI dose-dependently displaced [3H]-15S-(16-m-tolyl)isocarbacyclin on a rat brain slice.

L2 ANSWER 20 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 207283-63-4 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[(1E,3S)-4-(3-azido-5-methylphenyl)-3-hydroxy-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 6-[4-(3-azido-5-methylphenyl)-3-hydroxy-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]-
FS STEREOSEARCH
MF C25 H33 N3 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 129:4520 CA

TI Preparation of isocarbacyclin derivatives, their radiolabeled compounds, and their use as photoaffinity labeling probes
IN Watanabe, Yasuyoshi; Hasato, Atsuo; Watanabe, Yumiko; Suzuki, Masaki
PA Foundation for Scientific Technology Promotion, Japan; Hasato, Atsuo
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10087608	A2	19980407	JP 1996-243122	19960913
PRAI	JP 1996-243122	19960913			

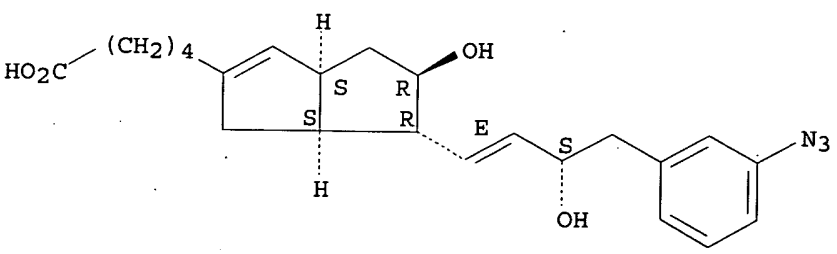
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The derivs. I (R1 = H, alkyl, cation; R2 = alkylene; R3 = H, Me) are prepd. by treatment of Horner-Emmons reagents II with formyl compds. III (R4 = C1-5 alkyl; R5 = H, tetrahydropyranyl) in the presence of bases, deprotection of OH-protective group if necessary, redn. of the resulting ketones IV, and hydrolysis if necessary. Also claimed are I labeled with 3H, 11C, or 14C at the arbitrary position and photoaffinity labeling using the radiolabeled I as probes, esp. for labeling of prostacyclin receptors. I are also useful as drugs for central nervous system disorders. A MeOH soln. of 16-(3-azidophenyl)-15-dehydro-17,18,19,20-tetranorisocarbacyclin Me ester prepd. from di-Me 2-oxo-3-(3-azidophenyl)propylphosphonate and III (R4 = Me, R5 = H), was treated with CeCl3.7H2O at room temp. then NaBH4 at 0.degree., and the resulting product was fractionated by silica gel chromatog. to give 48% 16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester and 49% 15-epi-16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester (V). A MeOH soln. of V was treated with an aq. NaOH soln. to give 96% free acid (VI). VI dose-dependently displaced [3H]-15S-(16-m-tolyl)isocarbacyclin on a rat brain slice.

L2 ANSWER 21 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 207283-54-3 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[(1E,3S)-4-(3-azidophenyl)-3-hydroxy-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 6-[4-(3-azidophenyl)-3-hydroxy-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]-
FS STEREOSEARCH
MF C23 H29 N3 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 129:4520 CA
TI Preparation of isocarbacyclin derivatives, their radiolabeled compounds, and their use as photoaffinity labeling probes
IN Watanabe, Yasuyoshi; Hasato, Atsuo; Watanabe, Yumiko; Suzuki, Masaki
PA Foundation for Scientific Technology Promotion, Japan; Hasato, Atsuo
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10087608	A2	19980407	JP 1996-243122	19960913
PRAI	JP 1996-243122		19960913		

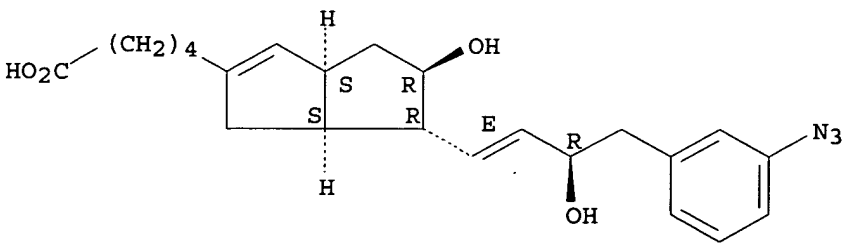
GI

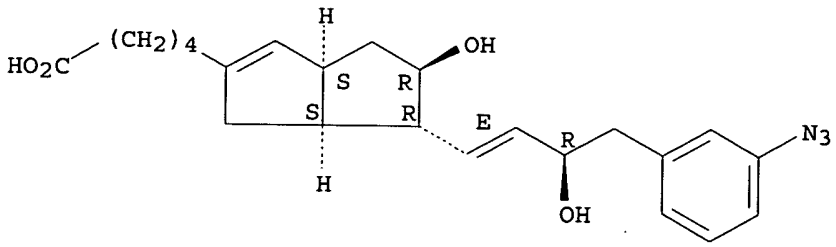
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The derivs. I (R1 = H, alkyl, cation; R2 = alkylene; R3 = H, Me) are prepd. by treatment of Horner-Emmons reagents II with formyl compds. III (R4 = C1-5 alkyl; R5 = H, tetrahydropyranyl) in the presence of bases, deprotection of OH-protective group if necessary, redn. of the resulting ketones IV, and hydrolysis if necessary. Also claimed are I labeled with 3H, 11C, or 14C at the arbitrary position and photoaffinity labeling using the radiolabeled I as probes, esp. for labeling of prostacyclin receptors. I are also useful as drugs for central nervous system disorders. A MeOH soln. of 16-(3-azidophenyl)-15-dehydro-17,18,19,20-tetranorisocarbacyclin Me ester prepd. from di-Me 2-oxo-3-(3-azidophenyl)propylphosphonate and III (R4 = Me, R5 = H), was treated with CeCl3.7H2O at room temp. then NaBH4 at 0.degree., and the resulting product was fractionated by silica gel chromatog. to give 48% 16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester and 49% 15-epi-16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester (V). A MeOH soln. of V was treated with an aq. NaOH soln. to give 96% free acid (VI). VI dose-dependently displaced [3H]-15S-(16-m-tolyl)isocarbacyclin on a rat brain slice.

L2 ANSWER 22 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 207283-51-0 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[(1E,3R)-4-(3-azidophenyl)-3-hydroxy-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 6-[4-(3-azidophenyl)-3-hydroxy-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]-
FS STEREOSEARCH
MF C23 H29 N3 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.





1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 129:4520 CA
TI Preparation of isocarbacyclin derivatives, their radiolabeled compounds, and their use as photoaffinity labeling probes
IN Watanabe, Yasuyoshi; Hasato, Atsuo; Watanabe, Yumiko; Suzuki, Masaki
PA Foundation for Scientific Technology Promotion, Japan; Hasato, Atsuo
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10087608	A2	19980407	JP 1996-243122	19960913
PRAI	JP 1996-243122	19960913			

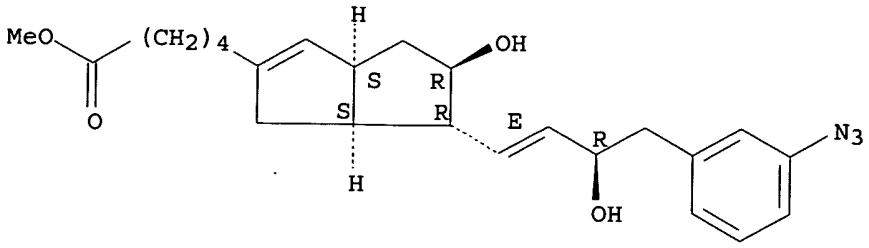
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The derivs. I (R1 = H, alkyl, cation; R2 = alkylene; R3 = H, Me) are prepd. by treatment of Horner-Emmons reagents II with formyl compds. III (R4 = C1-5 alkyl; R5 = H, tetrahydropyranyl) in the presence of bases, deprotection of OH-protective group if necessary, redn. of the resulting ketones IV, and hydrolysis if necessary. Also claimed are I labeled with 3H, 11C, or 14C at the arbitrary position and photoaffinity labeling using the radiolabeled I as probes, esp. for labeling of prostacyclin receptors. I are also useful as drugs for central nervous system disorders. A MeOH soln. of 16-(3-azidophenyl)-15-dehydro-17,18,19,20-tetranorisocarbacyclin Me ester prepd. from di-Me 2-oxo-3-(3-azidophenyl)propylphosphonate and III (R4 = Me, R5 = H), was treated with CeCl3.7H2O at room temp. then NaBH4 at 0.degree., and the resulting product was fractionated by silica gel chromatog. to give 48% 16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester and 49% 15-epi-16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester (V). A MeOH soln. of V was treated with an aq. NaOH soln. to give 96% free acid (VI). VI dose-dependently displaced [3H]-15S-(16-m-tolyl)isocarbacyclin on a rat brain slice.

L2 ANSWER 23 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 207283-48-5 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[(1E,3R)-4-(3-azidophenyl)-3-hydroxy-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 6-[4-(3-azidophenyl)-3-hydroxy-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]-
FS STEREOSEARCH
MF C24 H31 N3 O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 129:4520 CA
TI Preparation of isocarbacyclin derivatives, their radiolabeled compounds, and their use as photoaffinity labeling probes
IN Watanabe, Yasuyoshi; Hasato, Atsuo; Watanabe, Yumiko; Suzuki, Masaki
PA Foundation for Scientific Technology Promotion, Japan; Hasato, Atsuo
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10087608	A2	19980407	JP 1996-243122	19960913
PRAI	JP 1996-243122		19960913		

GI

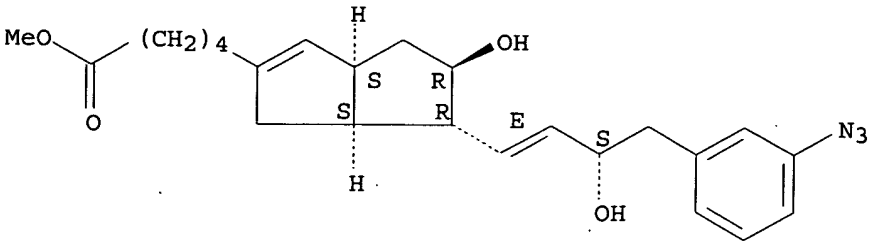
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The derivs. I (R1 = H, alkyl, cation; R2 = alkylene; R3 = H, Me) are prepd. by treatment of Horner-Emmons reagents II with formyl compds. III (R4 = C1-5 alkyl; R5 = H, tetrahydropyranyl) in the presence of bases, deprotection of OH-protective group if necessary, redn. of the resulting ketones IV, and hydrolysis if necessary. Also claimed are I labeled with 3H, 11C, or 14C at the arbitrary position and photoaffinity labeling using the radiolabeled I as probes, esp. for labeling of prostacyclin receptors. I are also useful as drugs for central nervous system disorders. A MeOH soln. of 16-(3-azidophenyl)-15-dehydro-17,18,19,20-tetranorisocarbacyclin Me ester prepd. from di-Me 2-oxo-3-(3-azidophenyl)propylphosphonate and III (R4 = Me, R5 = H), was treated with CeCl3.7H2O at room temp. then NaBH4 at 0.degree., and the resulting product was fractionated by silica gel chromatog. to give 48% 16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester and 49% 15-epi-16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester (V). A MeOH soln. of V was treated with an aq. NaOH soln. to give 96% free acid (VI). VI dose-dependently displaced [3H]-15S-(16-m-tolyl)isocarbacyclin on a rat brain slice.

L2 ANSWER 24 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 207283-43-0 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[(1E,3S)-4-(3-azidophenyl)-3-hydroxy-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 6-[4-(3-azidophenyl)-3-hydroxy-1-butenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]-

FS STEREOSEARCH
MF C24 H31 N3 O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 129:4520 CA
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IN Watanabe, Yasuyoshi; Hasato, Atsuo; Watanabe, Yumiko; Suzuki, Masaki
PA Foundation for Scientific Technology Promotion, Japan; Hasato, Atsuo
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10087608	A2	19980407	JP 1996-243122	19960913
PRAI	JP 1996-243122		19960913		

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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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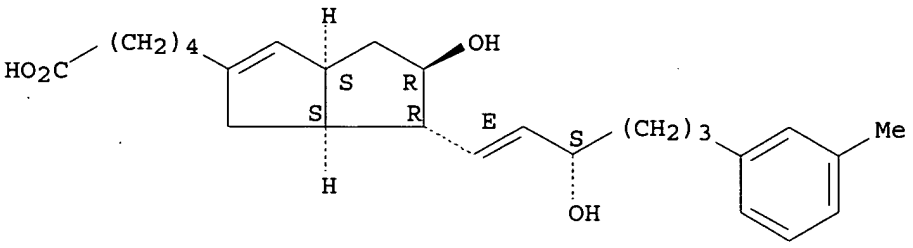
L2 ANSWER 25 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 184866-49-7 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E,3S)-3-hydroxy-6-(3-methylphenyl)-1-hexenyl]-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-6-(3-methylphenyl)-1-hexenyl]-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]-
FS STEREOSEARCH
MF C26 H36 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:139854 CA
TI A novel subtype of prostacyclin receptor in the central nervous system
AU Watanabe, Yumiko; Matsumura, Kiyoshi; Takechi, Hajime; Kato, Koichi; Morii, Hiroshi; Bjorkman, Margareta; Langstrom, Bengt; Noyori, Ryoji; Suzuki, Masaaki; Watanabe, Yasuyoshi
CS Subfemtomole Biorecognition Project, ICORP, Department of Neuroscience, Osaka Bioscience Institute, Japan Science and Technology Corporation, Osaka, 565-0874, Japan
SO Journal of Neurochemistry (1999), 72(6), 2583-2592
CODEN: JONRA9; ISSN: 0022-3042
PB Lippincott Williams & Wilkins
DT Journal
LA English
AB Recently, in the course of the authors' search for the prostacyclin receptor in the brain, the authors found a novel subtype, designated as IP2, which was finely discriminated by use of the specific ligand (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (15R-TIC) and specifically localized in the rostral part of the brain. In the present study, the tritiated compd. 15R-[15-3H]TIC was synthesized and utilized for more specific research on IP2. The specificity of binding to rat brain regions was confirmed by use of several prostacyclin derivs. including 15S-TIC. Mapping of 15R- and 15S-[3H]TIC binding in adjacent pairs of frozen sections of rat brain demonstrated a quite similar pattern of distribution in almost all rostral brain regions, indicating that the regions may contain only the IP2 subtype. 15R-[3H]TIC binding was very faint as compared with 15S-[3H]TIC binding in the caudal medullary region. High densities of 15R-[3H]TIC binding sites were shown in the dorsal part of the lateral septal nucleus, thalamic nuclei, limbic structures, and some of the cortical regions. Scatchard plot anal. showed two components of high-affinity 15R-[3H]TIC binding in the rostral regions, one with a KD value at .apprx.1 nM and the other with .apprx.30 nM. These results strengthen the authors' previous finding that a different subtype of prostacyclin receptor is expressed in the CNS, and the map with 15R-[3H]TIC obtained here could guide further studies on the mol. and functional properties of the IP2.
RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

AN 126:59803 CA
TI Isocarbacyclin derivatives
IN Watanabe, Yasuyoshi; Suzuki, Masaaki; Hazato, Atsuo; Langstrom, Bengt
PA Research Development Corporation of Japan, Japan
SO Can. Pat. Appl., 39 pp.
CODEN: CPXXEB
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 2168514	AA	19960911	CA 1996-2168514	19960131
	JP 08245498	A2	19960924	JP 1995-51589	19950310
	JP 3250936	B2	20020128		
	JP 2002128730	A2	20020509	JP 2001-250732	19950310
	US 5700833	A	19971223	US 1996-594152	19960131
PRAI	JP 1995-51589	19950310			

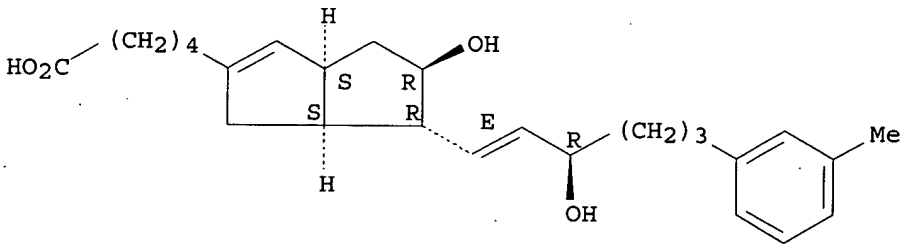
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention provides novel isocarbacyclin derivs. I [R = H, alkyl, cation; X = alkylene] useful for search and study of the prostacyclin receptor and as a therapeutic drug for central nervous system diseases. Thus, 13,14-dihydroxy-13,14-dihydroisocarbacyclin Me ester was oxidized with NaIO4 and treated with 3-MeC6H4CH2COCH2P(O)(OMe)2, followed by redn. and ester hydrolysis to give the acid II. II bound to both thalamic and medulla oblongata nuclear prostacyclin receptors but showed no platelet aggregation inhibiting activity.

L2 ANSWER 26 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 184866-48-6 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E,3R)-3-hydroxy-6-(3-methylphenyl)-1-hexenyl]-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-6-(3-methylphenyl)-1-hexenyl]-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]-
FS STEREOSEARCH
MF C26 H36 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



102

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:139854 CA
TI A novel subtype of prostacyclin receptor in the central nervous system
AU Watanabe, Yumiko; Matsumura, Kiyoshi; Takechi, Hajime; Kato, Koichi; Morii, Hiroshi; Bjorkman, Margareta; Langstrom, Bengt; Noyori, Ryoji; Suzuki, Masaaki; Watanabe, Yasuyoshi
CS Subfemtomole Biorecognition Project, ICORP, Department of Neuroscience, Osaka Bioscience Institute, Japan Science and Technology Corporation, Osaka, 565-0874, Japan
SO Journal of Neurochemistry (1999), 72(6), 2583-2592
CODEN: JONRA9; ISSN: 0022-3042
PB Lippincott Williams & Wilkins
DT Journal
LA English
AB Recently, in the course of the authors' search for the prostacyclin receptor in the brain, the authors found a novel subtype, designated as IP2, which was finely discriminated by use of the specific ligand (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (15R-TIC) and specifically localized in the rostral part of the brain. In the present study, the tritiated compd. 15R-[15-3H]TIC was synthesized and utilized for more specific research on IP2. The specificity of binding to rat brain regions was confirmed by use of several prostacyclin derivs. including 15S-TIC. Mapping of 15R- and 15S-[3H]TIC binding in adjacent pairs of frozen sections of rat brain demonstrated a quite similar pattern of distribution in almost all rostral brain regions, indicating that the regions may contain only the IP2 subtype. 15R-[3H]TIC binding was very faint as compared with 15S-[3H]TIC binding in the caudal medullary region. High densities of 15R-[3H]TIC binding sites were shown in the dorsal part of the lateral septal nucleus, thalamic nuclei, limbic structures, and some of the cortical regions. Scatchard plot anal. showed two components of high-affinity 15R-[3H]TIC binding in the rostral regions, one with a KD value at .apprx.1 nM and the other with .apprx.30 nM. These results strengthen the authors' previous finding that a different subtype of prostacyclin receptor is expressed in the CNS, and the map with 15R-[3H]TIC obtained here could guide further studies on the mol. and functional properties of the IP2.
RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

AN 126:59803 CA
TI Isocarbacyclin derivatives
IN Watanabe, Yasuyoshi; Suzuki, Masaaki; Hazato, Atsuo; Langstrom, Bengt
PA Research Development Corporation of Japan, Japan
SO Can. Pat. Appl., 39 pp.
CODEN: CPXXEB
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 2168514	AA	19960911	CA 1996-2168514	19960131
	JP 08245498	A2	19960924	JP 1995-51589	19950310
	JP 3250936	B2	20020128		
	JP 2002128730	A2	20020509	JP 2001-250732	19950310
	US 5700833	A	19971223	US 1996-594152	19960131
PRAI	JP 1995-51589	19950310			

GI

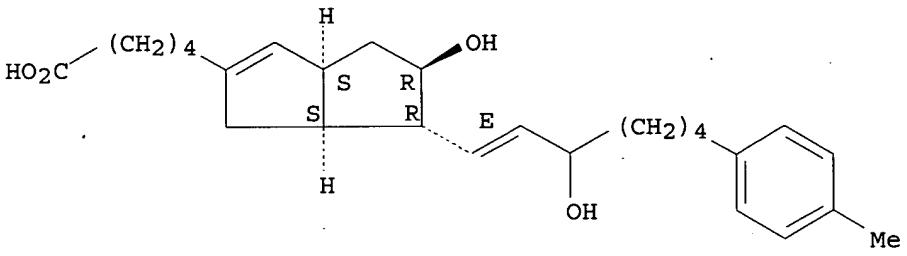
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention provides novel isocarbacyclin derivs. I [R = H, alkyl, cation; X = alkylene] useful for search and study of the prostacyclin receptor and as a therapeutic drug for central nervous system

diseases. Thus, 13,14-dihydroxy-13,14-dihydroisocarbacyclin Me ester was oxidized with NaIO4 and treated with 3-MeC6H4CH2COCH2P(O)(OMe)2, followed by redn. and ester hydrolysis to give the acid II. II bound to both thalamic and medulla oblongata nuclear prostacyclin receptors but showed no platelet aggregation inhibiting activity.

L2 ANSWER 27 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 184866-47-5 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E)-3-hydroxy-7-(4-methylphenyl)-1-heptenyl]-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-7-(4-methylphenyl)-1-heptenyl]-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E),6a.alpha.]]-[partial]-
FS STEREOSEARCH
MF C27 H38 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:139854 CA
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AU Watanabe, Yumiko; Matsumura, Kiyoshi; Takechi, Hajime; Kato, Koichi; Morii, Hiroshi; Bjorkman, Margareta; Langstrom, Bengt; Noyori, Ryoji; Suzuki, Masaaki; Watanabe, Yasuyoshi
CS Subfemtomole Biorecognition Project, ICORP, Department of Neuroscience, Osaka Bioscience Institute, Japan Science and Technology Corporation, Osaka, 565-0874, Japan
SO Journal of Neurochemistry (1999), 72(6), 2583-2592
CODEN: JONRA9; ISSN: 0022-3042
PB Lippincott Williams & Wilkins
DT Journal
LA English
AB Recently, in the course of the authors' search for the prostacyclin receptor in the brain, the authors found a novel subtype, designated as IP2, which was finely discriminated by use of the specific ligand (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (15R-TIC) and specifically localized in the rostral part of the brain. In the present study, the tritiated compd. 15R-[15-3H]TIC was synthesized and utilized for more specific research on IP2. The specificity of binding to rat brain regions was confirmed by use of several prostacyclin derivs. including 15S-TIC. Mapping of 15R- and 15S-[3H]TIC binding in adjacent pairs of frozen sections of rat brain demonstrated a quite similar pattern of distribution in almost all rostral brain regions, indicating that the regions may contain only the IP2 subtype. 15R-[3H]TIC binding was very faint as compared with 15S-[3H]TIC binding in the caudal medullary region. High densities of 15R-[3H]TIC binding sites were shown in the dorsal part

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RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

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PA Research Development Corporation of Japan, Japan
SO Can. Pat. Appl., 39 pp.
CODEN: CPXXEB
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 2168514	AA	19960911	CA 1996-2168514	19960131
	JP 08245498	A2	19960924	JP 1995-51589	19950310
	JP 3250936	B2	20020128		
	JP 2002128730	A2	20020509	JP 2001-250732	19950310
	US 5700833	A	19971223	US 1996-594152	19960131
PRAI	JP 1995-51589	19950310			

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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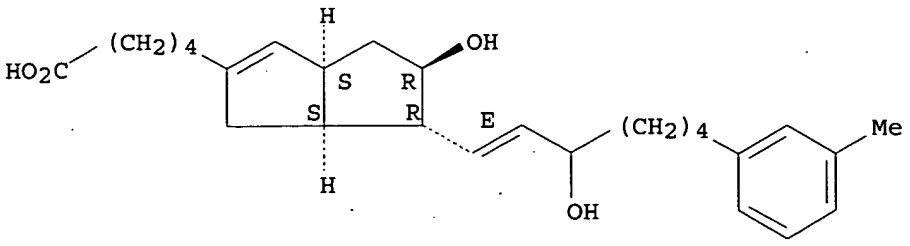
L2 ANSWER 28 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 184866-46-4 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E)-3-hydroxy-7-(3-methylphenyl)-1-heptenyl]-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-7-(3-methylphenyl)-1-heptenyl]-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E),6a.alpha.]]-[partial]-
FS STEREOSEARCH
MF C27 H38 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:139854 CA
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AU Watanabe, Yumiko; Matsumura, Kiyoshi; Takechi, Hajime; Kato, Koichi; Morii, Hiroshi; Bjorkman, Margareta; Langstrom, Bengt; Noyori, Ryoji; Suzuki, Masaaki; Watanabe, Yasuyoshi
CS Subfemtomole Biorecognition Project, ICORP, Department of Neuroscience, Osaka Bioscience Institute, Japan Science and Technology Corporation, Osaka, 565-0874, Japan
SO Journal of Neurochemistry (1999), 72(6), 2583-2592
CODEN: JONRA9; ISSN: 0022-3042
PB Lippincott Williams & Wilkins
DT Journal
LA English
AB Recently, in the course of the authors' search for the prostacyclin receptor in the brain, the authors found a novel subtype, designated as IP2, which was finely discriminated by use of the specific ligand (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (15R-TIC) and specifically localized in the rostral part of the brain. In the present study, the tritiated compd. 15R-[15-3H]TIC was synthesized and utilized for more specific research on IP2. The specificity of binding to rat brain regions was confirmed by use of several prostacyclin derivs. including 15S-TIC. Mapping of 15R- and 15S-[3H]TIC binding in adjacent pairs of frozen sections of rat brain demonstrated a quite similar pattern of distribution in almost all rostral brain regions, indicating that the regions may contain only the IP2 subtype. 15R-[3H]TIC binding was very faint as compared with 15S-[3H]TIC binding in the caudal medullary region. High densities of 15R-[3H]TIC binding sites were shown in the dorsal part of the lateral septal nucleus, thalamic nuclei, limbic structures, and some of the cortical regions. Scatchard plot anal. showed two components of high-affinity 15R-[3H]TIC binding in the rostral regions, one with a KD value at .apprx.1 nM and the other with .apprx.30 nM. These results strengthen the authors' previous finding that a different subtype of prostacyclin receptor is expressed in the CNS, and the map with 15R-[3H]TIC obtained here could guide further studies on the mol. and functional properties of the IP2.
RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

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PA Research Development Corporation of Japan, Japan
SO Can. Pat. Appl., 39 pp.
CODEN: CPXXEB
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI	CA 2168514	AA	19960911	CA 1996-2168514	19960131
	JP 08245498	A2	19960924	JP 1995-51589	19950310
	JP 3250936	B2	20020128		
	JP 2002128730	A2	20020509	JP 2001-250732	19950310
	US 5700833	A	19971223	US 1996-594152	19960131
PRAI	JP 1995-51589	19950310			

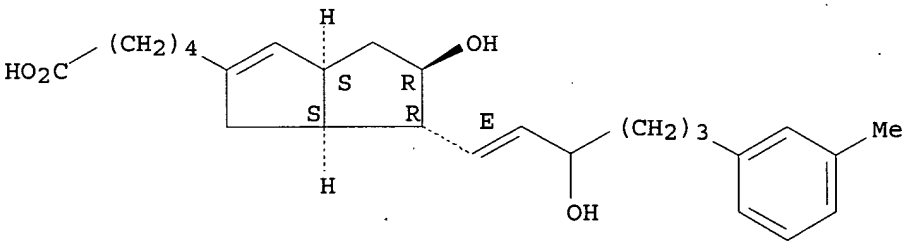
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention provides novel isocarbacyclin derivs. I [R = H, alkyl, cation; X = alkylene] useful for search and study of the prostacyclin receptor and as a therapeutic drug for central nervous system diseases. Thus, 13,14-dihydroxy-13,14-dihydroisocarbacyclin Me ester was oxidized with NaIO4 and treated with 3-MeC6H4CH2COCH2P(O)(OMe)2, followed by redn. and ester hydrolysis to give the acid II. II bound to both thalamic and medulla oblongata nuclear prostacyclin receptors but showed no platelet aggregation inhibiting activity.

L2 ANSWER 29 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 184866-45-3 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E)-3-hydroxy-6-(3-methylphenyl)-1-hexenyl]-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-6-(3-methylphenyl)-1-hexenyl]-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E),6a.alpha.]]-[partial]-
FS STEREOSEARCH
MF C26 H36 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:139854 CA
TI A novel subtype of prostacyclin receptor in the central nervous system
AU Watanabe, Yumiko; Matsumura, Kiyoshi; Takechi, Hajime; Kato, Koichi; Morii, Hiroshi; Bjorkman, Margareta; Langstrom, Bengt; Noyori, Ryoji; Suzuki, Masaaki; Watanabe, Yasuyoshi
CS Subfemtomole Biorecognition Project, ICORP, Department of Neuroscience, Osaka Bioscience Institute, Japan Science and Technology Corporation, Osaka, 565-0874, Japan
SO Journal of Neurochemistry (1999), 72(6), 2583-2592
CODEN: JONRA9; ISSN: 0022-3042

PB Lippincott Williams & Wilkins
DT Journal
LA English
AB Recently, in the course of the authors' search for the prostacyclin receptor in the brain, the authors found a novel subtype, designated as IP2, which was finely discriminated by use of the specific ligand. (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (15R-TIC) and specifically localized in the rostral part of the brain. In the present study, the tritiated compd. 15R-[15-3H]TIC was synthesized and utilized for more specific research on IP2. The specificity of binding to rat brain regions was confirmed by use of several prostacyclin derivs. including 15S-TIC. Mapping of 15R- and 15S-[3H]TIC binding in adjacent pairs of frozen sections of rat brain demonstrated a quite similar pattern of distribution in almost all rostral brain regions, indicating that the regions may contain only the IP2 subtype. 15R-[3H]TIC binding was very faint as compared with 15S-[3H]TIC binding in the caudal medullary region. High densities of 15R-[3H]TIC binding sites were shown in the dorsal part of the lateral septal nucleus, thalamic nuclei, limbic structures, and some of the cortical regions. Scatchard plot anal. showed two components of high-affinity 15R-[3H]TIC binding in the rostral regions, one with a KD value at .apprx.1 nM and the other with .apprx.30 nM. These results strengthen the authors' previous finding that a different subtype of prostacyclin receptor is expressed in the CNS, and the map with 15R-[3H]TIC obtained here could guide further studies on the mol. and functional properties of the IP2.
RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

AN 126:59803 CA
TI Isocarbacyclin derivatives
IN Watanabe, Yasuyoshi; Suzuki, Masaaki; Hazato, Atsuo; Langstrom, Bengt
PA Research Development Corporation of Japan, Japan
SO Can. Pat. Appl., 39 pp.
CODEN: CPXXEB
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 2168514	AA	19960911	CA 1996-2168514	19960131
	JP 08245498	A2	19960924	JP 1995-51589	19950310
	JP 3250936	B2	20020128		
	JP 2002128730	A2	20020509	JP 2001-250732	19950310
	US 5700833	A	19971223	US 1996-594152	19960131
PRAI	JP 1995-51589	19950310			

GI

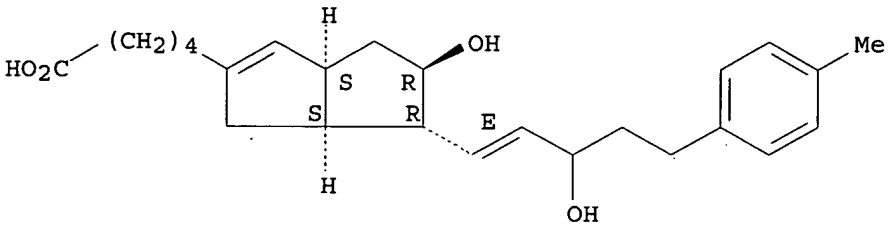
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention provides novel isocarbacyclin derivs. I [R = H, alkyl, cation; X = alkylene] useful for search and study of the prostacyclin receptor and as a therapeutic drug for central nervous system diseases. Thus, 13,14-dihydroxy-13,14-dihydroisocarbacyclin Me ester was oxidized with NaIO4 and treated with 3-MeC6H4CH2COCH2P(O)(OMe)2, followed by redn. and ester hydrolysis to give the acid II. II bound to both thalamic and medulla oblongata nuclear prostacyclin receptors but showed no platelet aggregation inhibiting activity.

L2 ANSWER 30 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 184866-44-2 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E)-3-hydroxy-5-(4-methylphenyl)-1-pentenyl]-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:

CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-5-(4-methylphenyl)-1-pentenyl]-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E),6a.alpha.]]-[partial]-
FS STEREOSEARCH
MF C25 H34 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:139854 CA
TI A novel subtype of prostacyclin receptor in the central nervous system
AU Watanabe, Yumiko; Matsumura, Kiyoshi; Takechi, Hajime; Kato, Koichi; Morii, Hiroshi; Bjorkman, Margareta; Langstrom, Bengt; Noyori, Ryoji; Suzuki, Masaaki; Watanabe, Yasuyoshi
CS Subfemtomole Biorecognition Project, ICORP, Department of Neuroscience, Osaka Bioscience Institute, Japan Science and Technology Corporation, Osaka, 565-0874, Japan
SO Journal of Neurochemistry (1999), 72(6), 2583-2592
CODEN: JONRA9; ISSN: 0022-3042
PB Lippincott Williams & Wilkins
DT Journal
LA English
AB Recently, in the course of the authors' search for the prostacyclin receptor in the brain, the authors found a novel subtype, designated as IP2, which was finely discriminated by use of the specific ligand (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (15R-TIC) and specifically localized in the rostral part of the brain. In the present study, the tritiated compd. 15R-[15-3H]TIC was synthesized and utilized for more specific research on IP2. The specificity of binding to rat brain regions was confirmed by use of several prostacyclin derivs. including 15S-TIC. Mapping of 15R- and 15S-[3H]TIC binding in adjacent pairs of frozen sections of rat brain demonstrated a quite similar pattern of distribution in almost all rostral brain regions, indicating that the regions may contain only the IP2 subtype. 15R-[3H]TIC binding was very faint as compared with 15S-[3H]TIC binding in the caudal medullary region. High densities of 15R-[3H]TIC binding sites were shown in the dorsal part of the lateral septal nucleus, thalamic nuclei, limbic structures, and some of the cortical regions. Scatchard plot anal. showed two components of high-affinity 15R-[3H]TIC binding in the rostral regions, one with a KD value at .apprx.1 nM and the other with .apprx.30 nM. These results strengthen the authors' previous finding that a different subtype of prostacyclin receptor is expressed in the CNS, and the map with 15R-[3H]TIC obtained here could guide further studies on the mol. and functional properties of the IP2.
RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

AN 126:59803 CA
TI Isocarbacyclin derivatives
IN Watanabe, Yasuyoshi; Suzuki, Masaaki; Hazato, Atsuo; Langstrom, Bengt
PA Research Development Corporation of Japan, Japan
SO Can. Pat. Appl., 39 pp.
CODEN: CPXXEB
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 2168514	AA	19960911	CA 1996-2168514	19960131
	JP 08245498	A2	19960924	JP 1995-51589	19950310
	JP 3250936	B2	20020128		
	JP 2002128730	A2	20020509	JP 2001-250732	19950310
	US 5700833	A	19971223	US 1996-594152	19960131
PRAI	JP 1995-51589	19950310			

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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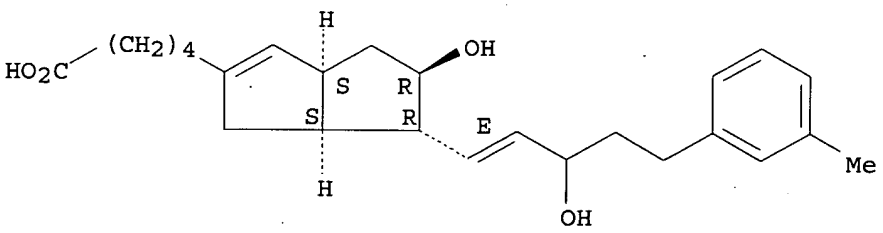
L2 ANSWER 31 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 184866-43-1 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E)-3-hydroxy-5-(3-methylphenyl)-1-pentenyl]-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-5-(3-methylphenyl)-1-pentenyl]-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E),6a.alpha.]]-[partial]-
FS STEREOSEARCH
MF C25 H34 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:139854 CA

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AU Watanabe, Yumiko; Matsumura, Kiyoshi; Takechi, Hajime; Kato, Koichi; Morii, Hiroshi; Bjorkman, Margareta; Langstrom, Bengt; Noyori, Ryoji; Suzuki, Masaaki; Watanabe, Yasuyoshi
CS Subfemtomole Biorecognition Project, ICORP, Department of Neuroscience, Osaka Bioscience Institute, Japan Science and Technology Corporation, Osaka, 565-0874, Japan
SO Journal of Neurochemistry (1999), 72(6), 2583-2592
CODEN: JONRA9; ISSN: 0022-3042
PB Lippincott Williams & Wilkins
DT Journal
LA English
AB Recently, in the course of the authors' search for the prostacyclin receptor in the brain, the authors found a novel subtype, designated as IP2, which was finely discriminated by use of the specific ligand (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (15R-TIC) and specifically localized in the rostral part of the brain. In the present study, the tritiated compd. 15R-[15-3H]TIC was synthesized and utilized for more specific research on IP2. The specificity of binding to rat brain regions was confirmed by use of several prostacyclin derivs. including 15S-TIC. Mapping of 15R- and 15S-[3H]TIC binding in adjacent pairs of frozen sections of rat brain demonstrated a quite similar pattern of distribution in almost all rostral brain regions, indicating that the regions may contain only the IP2 subtype. 15R-[3H]TIC binding was very faint as compared with 15S-[3H]TIC binding in the caudal medullary region. High densities of 15R-[3H]TIC binding sites were shown in the dorsal part of the lateral septal nucleus, thalamic nuclei, limbic structures, and some of the cortical regions. Scatchard plot anal. showed two components of high-affinity 15R-[3H]TIC binding in the rostral regions, one with a KD value at .apprx.1 nM and the other with .apprx.30 nM. These results strengthen the authors' previous finding that a different subtype of prostacyclin receptor is expressed in the CNS, and the map with 15R-[3H]TIC obtained here could guide further studies on the mol. and functional properties of the IP2.
RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

AN 126:59803 CA
TI Isocarbacyclin derivatives
IN Watanabe, Yasuyoshi; Suzuki, Masaaki; Hazato, Atsuo; Langstrom, Bengt
PA Research Development Corporation of Japan, Japan
SO Can. Pat. Appl., 39 pp.
CODEN: CPXXEB
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 2168514	AA	19960911	CA 1996-2168514	19960131
	JP 08245498	A2	19960924	JP 1995-51589	19950310
	JP 3250936	B2	20020128		
	JP 2002128730	A2	20020509	JP 2001-250732	19950310
	US 5700833	A	19971223	US 1996-594152	19960131
PRAI	JP 1995-51589	19950310			

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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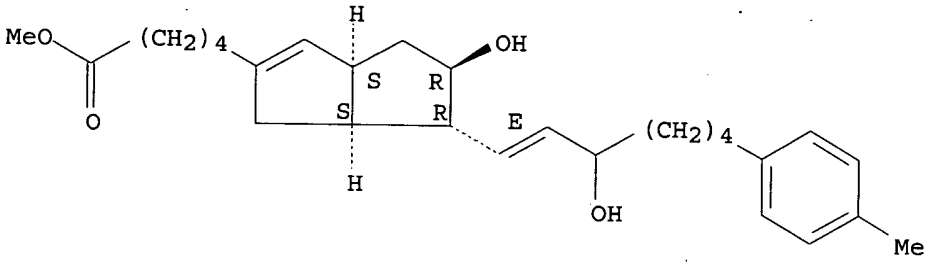
thalamic and medulla oblongata nuclear prostacyclin receptors but showed no platelet aggregation inhibiting activity.

L2 ANSWER 32 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 184866-42-0 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E)-3-hydroxy-7-(4-methylphenyl)-1-heptenyl]-, methyl ester, (3aS,5R,6R,6aS)-(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-7-(4-methylphenyl)-1-heptenyl]-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E),6a.alpha.]]-
FS STEREOSEARCH
MF C28 H40 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 126:59803 CA
TI Isocarbacyclin derivatives
IN Watanabe, Yasuyoshi; Suzuki, Masaaki; Hazato, Atsuo; Langstrom, Bengt
PA Research Development Corporation of Japan, Japan
SO Can. Pat. Appl., 39 pp.
CODEN: CPXXEB
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 2168514	AA	19960911	CA 1996-2168514	19960131
	JP 08245498	A2	19960924	JP 1995-51589	19950310
	JP 3250936	B2	20020128		
	JP 2002128730	A2	20020509	JP 2001-250732	19950310
	US 5700833	A	19971223	US 1996-594152	19960131
PRAI	JP 1995-51589	19950310			

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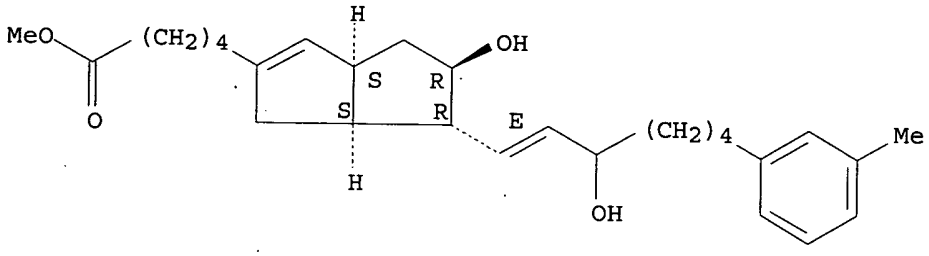
thalamic and medulla oblongata nuclear prostacyclin receptors but showed no platelet aggregation inhibiting activity.

L2 ANSWER 33 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 184866-41-9 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E)-3-hydroxy-7-(3-methylphenyl)-1-heptenyl]-, methyl ester, (3aS,5R,6R,6aS)-(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-7-(3-methylphenyl)-1-heptenyl]-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E),6a.alpha.]]-[partial]-
FS STEREOSEARCH
MF C28 H40 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 126:59803 CA
TI Isocarbacyclin derivatives
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PA Research Development Corporation of Japan, Japan
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DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 2168514	AA	19960911	CA 1996-2168514	19960131
	JP 08245498	A2	19960924	JP 1995-51589	19950310
	JP 3250936	B2	20020128		
	JP 2002128730	A2	20020509	JP 2001-250732	19950310
	US 5700833	A	19971223	US 1996-594152	19960131
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GI

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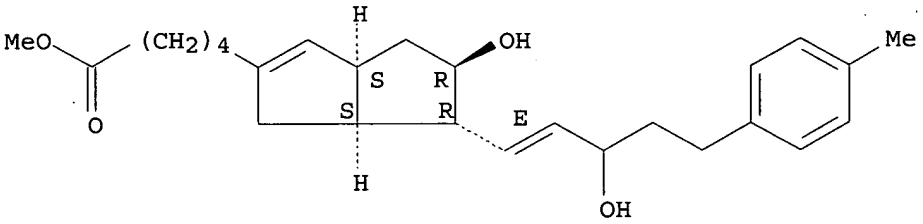
thalamic and medulla oblongata nuclear prostacyclin receptors but showed no platelet aggregation inhibiting activity.

L2 ANSWER 34 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 184866-40-8 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E)-3-hydroxy-5-(4-methylphenyl)-1-pentenyl]-, methyl ester, (3aS,5R,6R,6aS)-(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-5-(4-methylphenyl)-1-pentenyl]-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E),6a.alpha.]]-[partial]-
FS STEREOSEARCH
MF C26 H36 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
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REFERENCE 1

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SO Can. Pat. Appl., 39 pp.
CODEN: CPXXEB
DT Patent
LA English
FAN.CNT 1

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	JP 3250936	B2	20020128		
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GI

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L2 ANSWER 35 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 184866-39-5 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E)-3-hydroxy-5-(3-methylphenyl)-1-pentenyl]-, methyl ester, (3aS,5R,6R,6aS)-(9CI) (CA INDEX NAME)
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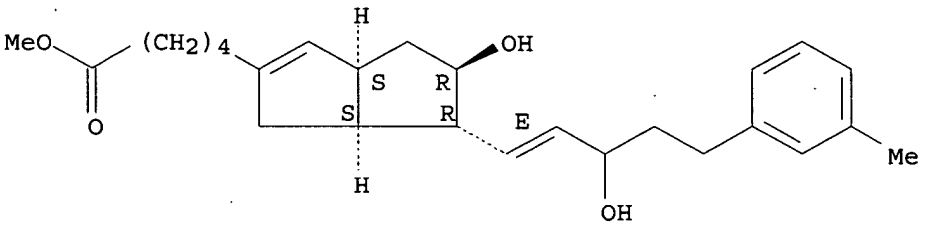
FS STEREOSEARCH
MF C26 H36 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 126:59803 CA
TI Isocarbacyclin derivatives
IN Watanabe, Yasuyoshi; Suzuki, Masaaki; Hazato, Atsuo; Langstrom, Bengt
PA Research Development Corporation of Japan, Japan
SO Can. Pat. Appl., 39 pp.
CODEN: CPXXEB
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 2168514	AA	19960911	CA 1996-2168514	19960131
	JP 08245498	A2	19960924	JP 1995-51589	19950310
	JP 3250936	B2	20020128		
	JP 2002128730	A2	20020509	JP 2001-250732	19950310
	US 5700833	A	19971223	US 1996-594152	19960131
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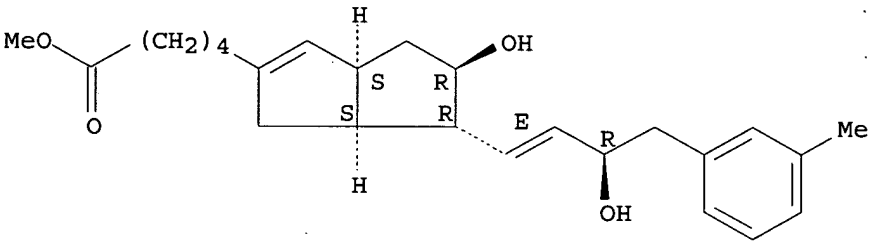
L2 ANSWER 36 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 175275-99-7 REGISTRY
CN 2-Pentalenepentanoic acid, 3,3a,4,5,6,6a-hexahydro-5-hydroxy-4-[(1E,3R)-3-hydroxy-4-(3-methylphenyl)-1-butenyl]-, methyl ester, (3aS,4R,5R,6aS)-(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-4-(3-methylphenyl)-1-butenyl]-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]-
FS STEREOSEARCH
MF C25 H34 O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

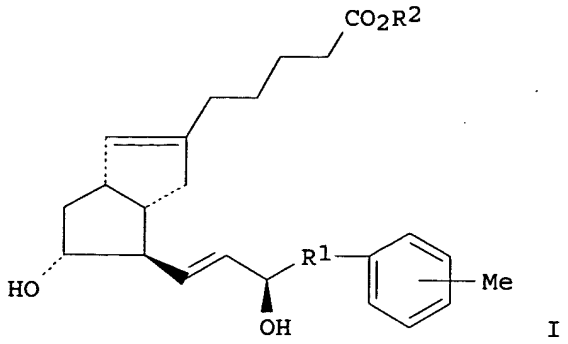
4 REFERENCES IN FILE CA (1957 TO DATE)
4 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 134:157581 CA
TI Neuropathy remedies
IN Suwa, Yorimasa; Yoshioka, Noboru; Arai, Takami; Sakurai, Katsutoshi; Suzuki, Jun; Watanabe, Yasuyoshi; Suzuki, Masaaki; Satoh, Takumi; Watanabe, Yumiko; Kataoka, Yosuke
PA Teijin Ltd., Japan; Osaka Bioscience Institute
SO PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001010445	A1	20010215	WO 2000-JP5267	20000804
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1208841	A1	20020529	EP 2000-950011	20000804
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
PRAI	JP 1999-222311		19990805		
	WO 2000-JP5267		20000804		

GI



I

AB Remedies for nerve degeneration diseases contg. as the active ingredient (15R)-isocarbacyclin derivs. of general formula [I] or 15-deoxyisocarbacyclin derivs. In formula I, R1 is C1-C6 alkylene; and R2 is hydrogen, C1-C7 alkyl, or a protective group.

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

AN 134:41988 CA

TI Rapid Methylation for the Synthesis of a 11C-Labeled Tolylisocarbacyclin Imaging the IP2 Receptor in a Living Human Brain

AU Suzuki, M.; Doi, H.; Kato, K.; Bjorkman, M.; Langstrom, B.; Watanabe, Y.; Noyori, R.

CS Faculty of Engineering, Department of Biomolecular Science, Gifu University, Gifu, 501-1193, Japan

SO Tetrahedron (2000), 56(42), 8263-8273
CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier Science Ltd.

DT Journal

LA English

AB A rapid method for Pd-promoted cross-coupling of Me iodide and tributyltin derivs. of tolylisocarbacyclins was developed with the objective of applying to the PET study on the IP2 receptor in a living human brain. The high efficiency is obtainable for both of the one-pot operation using a large excess of CuCl and the stepwise operation consisting of the initial prepn. of a methylpalladium complex followed by mixing with the remaining requisite materials for the cross-coupling. The latter protocol allowed for the highly reproducible synthesis of an actual PET tracer with total radioactivity of several GBq. Several stannanes could be employed as precursors of PET tracers in this rapid cross-coupling reaction.

RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 3

AN 126:59803 CA

TI Isocarbacyclin derivatives

IN Watanabe, Yasuyoshi; Suzuki, Masaaki; Hazato, Atsuo; Langstrom, Bengt

PA Research Development Corporation of Japan, Japan

SO Can. Pat. Appl., 39 pp.
CODEN: CPXXEB

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 2168514	AA	19960911	CA 1996-2168514	19960131
	JP 08245498	A2	19960924	JP 1995-51589	19950310
	JP 3250936	B2	20020128		
	JP 2002128730	A2	20020509	JP 2001-250732	19950310
	US 5700833	A	19971223	US 1996-594152	19960131
PRAI	JP 1995-51589	19950310			

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention provides novel isocarbacyclin derivs. I [R = H, alkyl, cation; X = alkylene] useful for search and study of the prostacyclin receptor and as a therapeutic drug for central nervous system diseases. Thus, 13,14-dihydroxy-13,14-dihydroisocarbacyclin Me ester was oxidized with NaIO4 and treated with 3-MeC6H4CH2COCH2P(O)(OMe)2, followed by redn. and ester hydrolysis to give the acid II. II bound to both thalamic and medulla oblongata nuclear prostacyclin receptors but showed no platelet aggregation inhibiting activity.

REFERENCE 4

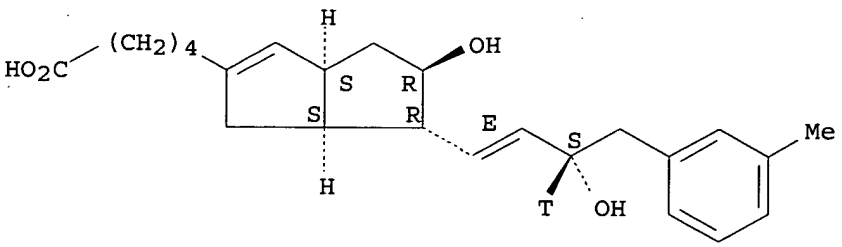
AN 124:260630 CA
TI (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin: A stable ligand with high binding affinity and selectivity for a prostacyclin receptor in the central nervous system
AU Suzuki, Masaaki; Kato, Koichi; Noyori, Ryoji; Watanabe, Yumiko; Takechi, Hajime; Matsumura, Kiyoshi; Langstroem, Bengt; Watanabe, Yasuyoshi
CS Dep. Applied Chemistry, Gifu Univ., Gifu, 501-11, Japan
SO Angewandte Chemie, International Edition in English (1996), 35(3), 334-36
CODEN: ACIEAY; ISSN: 0570-0833
PB VCH
DT Journal
LA English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compd. I was devised based on the the structural modification of the .omega. side chain of isocarbacyclin (II), a chem. stable PGI2 agonist, starting from the aldehyde intermediate III.

L2 ANSWER 37 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 175275-98-6 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E,3S)-3-hydroxy-4-(3-methylphenyl)-1-butenyl-3-t]-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-4-(3-methylphenyl)-1-butenyl-3-t]-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]-
FS STEREOSEARCH
MF C24 H31 O4 T
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



2 REFERENCES IN FILE CA (1957 TO DATE)

2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:139854 CA
TI A novel subtype of prostacyclin receptor in the central nervous system
AU Watanabe, Yumiko; Matsumura, Kiyoshi; Takechi, Hajime; Kato, Koichi; Morii, Hiroshi; Bjorkman, Margareta; Langstrom, Bengt; Noyori, Ryoji; Suzuki, Masaaki; Watanabe, Yasuyoshi
CS Subfemtomole Biorecognition Project, ICORP, Department of Neuroscience, Osaka Bioscience Institute, Japan Science and Technology Corporation, Osaka, 565-0874, Japan
SO Journal of Neurochemistry (1999), 72(6), 2583-2592
CODEN: JONRA9; ISSN: 0022-3042
PB Lippincott Williams & Wilkins
DT Journal
LA English
AB Recently, in the course of the authors' search for the prostacyclin receptor in the brain, the authors found a novel subtype, designated as IP2, which was finely discriminated by use of the specific ligand (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (15R-TIC) and specifically localized in the rostral part of the brain. In the present study, the tritiated compd. 15R-[15-3H]TIC was synthesized and utilized for more specific research on IP2. The specificity of binding to rat brain regions was confirmed by use of several prostacyclin derivs. including 15S-TIC. Mapping of 15R- and 15S-[3H]TIC binding in adjacent pairs of frozen sections of rat brain demonstrated a quite similar pattern of distribution in almost all rostral brain regions, indicating that the regions may contain only the IP2 subtype. 15R-[3H]TIC binding was very faint as compared with 15S-[3H]TIC binding in the caudal medullary region. High densities of 15R-[3H]TIC binding sites were shown in the dorsal part of the lateral septal nucleus, thalamic nuclei, limbic structures, and some of the cortical regions. Scatchard plot anal. showed two components of high-affinity 15R-[3H]TIC binding in the rostral regions, one with a KD value at .apprx.1 nM and the other with .apprx.30 nM. These results strengthen the authors' previous finding that a different subtype of prostacyclin receptor is expressed in the CNS, and the map with 15R-[3H]TIC obtained here could guide further studies on the mol. and functional properties of the IP2.
RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

AN 124:260630 CA
TI (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin: A stable ligand with high binding affinity and selectivity for a prostacyclin receptor in the central nervous system
AU Suzuki, Masaaki; Kato, Koichi; Noyori, Ryoji; Watanabe, Yumiko; Takechi, Hajime; Matsumura, Kiyoshi; Langstroem, Bengt; Watanabe, Yasuyoshi
CS Dep. Applied Chemistry, Gifu Univ., Gifu, 501-11, Japan
SO Angewandte Chemie, International Edition in English (1996), 35(3), 334-36
CODEN: ACIEAY; ISSN: 0570-0833
PB VCH
DT Journal
LA English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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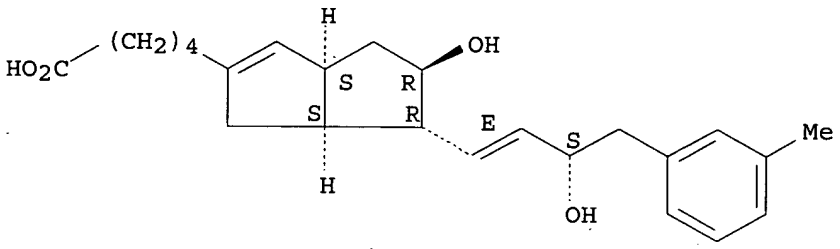
L2 ANSWER 38 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 175275-97-5 REGISTRY

CN 2-Pentalenepentanoic acid, 3,3a,4,5,6,6a-hexahydro-5-hydroxy-4-[(1E,3S)-3-hydroxy-4-(3-methylphenyl)-1-butenyl]-, (3aS,4R,5R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-4-(3-methylphenyl)-1-butenyl]-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]-
OTHER NAMES:
CN (15S)-TIC
FS STEREOSEARCH
MF C24 H32 O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
6 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 134:173045 CA
TI Neuropathy improvers containing nitrogenous compounds as the active ingredient
IN Sugiura, Satoshi; Tsutsumi, Takaharu; Suwa, Yorimasa; Arai, Takami; Sakurai, Katsutoshi; Yoshioka, Noboru; Tanokura, Akira; Suzuki, Jun
PA Teijin Limited, Japan
SO PCT Int. Appl., 429 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001010433	A1	20010215	WO 2000-JP5287	20000807
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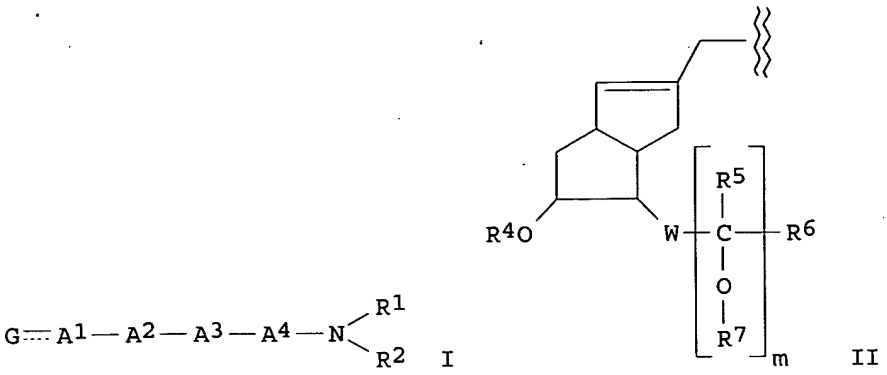
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1201235	A1	20020502	EP 2000-950027	20000807
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	BR 2000012907	A	20020611	BR 2000-12907	20000807
PRAI	JP 1999-222259	19990805			
	JP 1999-222260	19990805			
	WO 2000-JP5287	20000807			

GI



AB Compds. represented by general formula (I); and neuropathy improvers contg. the same as the active ingredient: wherein G is a group represented by the general formula (II) or the like: [wherein R4 is hydrogen, acyl, or the like; W is a single bond, alkylene, or the like; m is 0 or 1; R5 and R6 are each hydrogen, an aliph. hydrocarbon group, an alicyclic hydrocarbon group, an arom. hydrocarbon group, a heterocyclic group, or the like; and R7 is hydrogen, acyl, alkoxycarbonyl, or the like]; A2 is a single bond, -O-, -NR3-, or -S(=O)n-; A1 and A3 are each a single bond, an aliph. hydrocarbon group, an alicyclic hydrocarbon group, a heterocyclic group, phenylene, or the like; A4 is a single bond, carbonyl, an aliph. hydrocarbon group, or the like; and R1 and R2 are each hydrogen, alkyl, cycloalkyl, Ph, a heterocyclic group, or the like, these groups being each optionally substituted.

RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

AN 131:139854 CA
TI A novel subtype of prostacyclin receptor in the central nervous system
AU Watanabe, Yumiko; Matsumura, Kiyoshi; Takechi, Hajime; Kato, Koichi; Morii, Hiroshi; Bjorkman, Margareta; Langstrom, Bengt; Noyori, Ryoji; Suzuki, Masaaki; Watanabe, Yasuyoshi
CS Subfemtomole Biorecognition Project, ICORP, Department of Neuroscience, Osaka Bioscience Institute, Japan Science and Technology Corporation, Osaka, 565-0874, Japan
SO Journal of Neurochemistry (1999), 72(6), 2583-2592
CODEN: JONRA9; ISSN: 0022-3042
PB Lippincott Williams & Wilkins
DT Journal
LA English
AB Recently, in the course of the authors' search for the prostacyclin receptor in the brain, the authors found a novel subtype, designated as IP2, which was finely discriminated by use of the specific ligand (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (15R-TIC) and specifically localized in the rostral part of the brain. In the present study, the tritiated compd. 15R-[15-3H]TIC was synthesized and utilized for more specific research on IP2. The specificity of binding to rat brain regions was confirmed by use of several prostacyclin derivs. including 15S-TIC. Mapping of 15R- and 15S-[3H]TIC binding in adjacent pairs of frozen sections of rat brain demonstrated a quite similar pattern of distribution in almost all rostral brain regions, indicating that the regions may contain only the IP2 subtype. 15R-[3H]TIC binding was very faint as compared with 15S-[3H]TIC binding in the caudal medullary region. High densities of 15R-[3H]TIC binding sites were shown in the dorsal part of the lateral septal nucleus, thalamic nuclei, limbic structures, and some of the cortical regions. Scatchard plot anal. showed two components of high-affinity 15R-[3H]TIC binding in the rostral regions, one with a KD value at .apprx.1 nM and the other with .apprx.30 nM. These results strengthen the authors' previous finding that a different subtype of prostacyclin receptor is expressed in the CNS, and the map with 15R-[3H]TIC obtained here could guide further studies on the mol. and

functional properties of the IP2.
RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 3

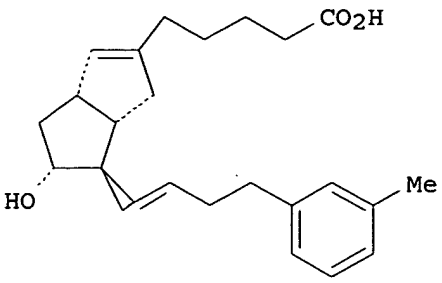
AN 131:129774 CA
TI Design of prostaglandins with high binding affinity and selectivity for an IP2 receptor in the central nervous system and their biological activity
AU Suzuki, Masaaki; Kato, Koichi; Noyori, Ryoji; Watanabe, Yumiko; Sato, Takumi; Matsumura, Kiyoshi; Watanabe, Yasuyoshi
CS Faculty of Engineering, Gifu University, Japan
SO Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1998), 40th, 145-150
CODEN: TYKYDS
PB Nippon Kagakkai
DT Journal
LA Japanese
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The role of prostacyclin (PGI2) in the central nervous system (CNS) has still been unclear because of the lack of a specific ligand for a PGI2 receptor in CNS. In this context, the authors recently elaborated 15R-TIC (I; R = OH, R1 = H) with high binding affinity and selectivity for novel IP2 receptor which is specifically expressed in CNS neurons. The R configuration of the hydroxy-bearing C(15) in 15R-TIC is fascinating, because, in general, the configuration of biol. active PGs at C(15) position is known to be S. In this symposium, the authors describe synthesis of the TIC derivs. for structure-binding affinity relationship in addn. to biol. actions. 15-Deoxy-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (I; R = R1 = H) (referred to as 15-deoxy-TIC) exhibited, among others, highest binding affinity and selectivity for a IP2 receptor. I (R = R1 = H) has been prepd. based on the combination of the Witting reaction and Pd(0)-mediated coupling of an allyl carbonate and a sulfone. Thus, Witting reaction of aldehyde II (R2 = CHO, R3 = THP) and a Ph3P:CHCHO led to II [R2 = (E)-CH:CHCHO, R3 = THP]. The redn. of this followed by methoxycarbonylation gave allyl carbonate II [R2 = (E)-CH:CHCH2-OCO2Me, R3 = THP] which was treated with disulfone III in the presence of a 1:1 mixt. of Pd(0) and diphenylphosphinoethane to give II [R2 = (E)-CH:CHCH2-C(SO2Ph)2C6H4Me-m, R3 = THP]. Reductive removal of Ph sulfonyl groups of this and subsequent deprotection gave II (R2 = CH2CH2C6H4Me-m, R3 = H), which was hydrolyzed to give I (R = R1 = H). I (R, R1 = OH, H; H, H) prevented apoptotic cell death of hippocampal neurons induced under high oxygen (50%) atm., whereas I (R = H, R1 = OH), isocarbacyclin, and natural PGs except for PGI2 did not show such a biol. effect.

REFERENCE 4

AN 130:325022 CA
TI 15-Deoxy-16-(m-tolyl)-17,18,19,20-tetranorisocarbacyclin: a simple TIC derivative with potent anti-apoptotic activity for neuronal cells
AU Suzuki, Masaaki; Kato, Koichi; Noyori, Ryoji; Watanabe, Yumiko; Satoh, Takumi; Matsumura, Kiyoshi; Watanabe, Yasuyoshi
CS Faculty of Engineering, Department of Biomolecular Science, Gifu University, Gifu, 501-1193, Japan
SO Chemical Communications (Cambridge) (1999), (4), 307-308
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
GI



I

AB Biol. remarkable 15-deoxy-TIC (I) has been realized by the removal of the C(15) chiral center in 15R-TIC, a stable ligand for a CNS-type prostacyclin receptor (IP2); this deoxy deriv. exhibits ten-fold higher affinity and selectivity than 15R-TIC for the IP2 receptor in correlation with the anti-apoptotic activity for neuronal cells.
RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 5

AN 126:59803 CA
TI Isocarbacyclin derivatives
IN Watanabe, Yasuyoshi; Suzuki, Masaaki; Hazato, Atsuo; Langstrom, Bengt
PA Research Development Corporation of Japan, Japan
SO Can. Pat. Appl., 39 pp.
CODEN: CPXXEB
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 2168514	AA	19960911	CA 1996-2168514	19960131
	JP 08245498	A2	19960924	JP 1995-51589	19950310
	JP 3250936	B2	20020128		
	JP 2002128730	A2	20020509	JP 2001-250732	19950310
	US 5700833	A	19971223	US 1996-594152	19960131
PRAI	JP 1995-51589	19950310			

GI

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REFERENCE 6

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AU Suzuki, Masaaki; Kato, Koichi; Noyori, Ryoji; Watanabe, Yumiko; Takechi, Hajime; Matsumura, Kiyoshi; Langstroem, Bengt; Watanabe, Yasuyoshi
CS Dep. Applied Chemistry, Gifu Univ., Gifu, 501-11, Japan
SO Angewandte Chemie, International Edition in English (1996), 35(3), 334-36
CODEN: ACIEAY; ISSN: 0570-0833

PB VCH
DT Journal
LA English
GI

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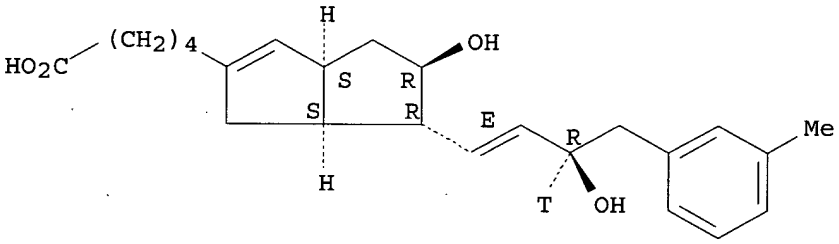
L2 ANSWER 39 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 175169-71-8 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E,3R)-3-hydroxy-4-(3-methylphenyl)-1-butenyl-3-t]-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-4-(3-methylphenyl)-1-butenyl-3-t]-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]-
OTHER NAMES:
CN [15-3H]-(15R)-TIC
FS STEREOSEARCH
MF C24 H31 O4 T
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



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1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
4 REFERENCES IN FILE CAPLUS (1957 TO DATE)

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TI A novel subtype of prostacyclin receptor in the central nervous system
AU Watanabe, Yumiko; Matsumura, Kiyoshi; Takechi, Hajime; Kato, Koichi; Morii, Hiroshi; Bjorkman, Margareta; Langstrom, Bengt; Noyori, Ryoji; Suzuki, Masaaki; Watanabe, Yasuyoshi
CS Subfemtomole Biorecognition Project, ICORP, Department of Neuroscience, Osaka Bioscience Institute, Japan Science and Technology Corporation, Osaka, 565-0874, Japan
SO Journal of Neurochemistry (1999), 72(6), 2583-2592
CODEN: JONRA9; ISSN: 0022-3042
PB Lippincott Williams & Wilkins
DT Journal
LA English
AB Recently, in the course of the authors' search for the prostacyclin receptor in the brain, the authors found a novel subtype, designated as IP2, which was finely discriminated by use of the specific ligand (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (15R-TIC) and specifically localized in the rostral part of the brain. In the present study, the tritiated compd. 15R-[15-3H]TIC was synthesized and utilized

for more specific research on IP2. The specificity of binding to rat brain regions was confirmed by use of several prostacyclin derivs. including 15S-TIC. Mapping of 15R- and 15S-[3H]TIC binding in adjacent pairs of frozen sections of rat brain demonstrated a quite similar pattern of distribution in almost all rostral brain regions, indicating that the regions may contain only the IP2 subtype. 15R-[3H]TIC binding was very faint as compared with 15S-[3H]TIC binding in the caudal medullary region. High densities of 15R-[3H]TIC binding sites were shown in the dorsal part of the lateral septal nucleus, thalamic nuclei, limbic structures, and some of the cortical regions. Scatchard plot anal. showed two components of high-affinity 15R-[3H]TIC binding in the rostral regions, one with a KD value at .apprx.1 nM and the other with .apprx.30 nM. These results strengthen the authors' previous finding that a different subtype of prostacyclin receptor is expressed in the CNS, and the map with 15R-[3H]TIC obtained here could guide further studies on the mol. and functional properties of the IP2.

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

AN 131:129774 CA
TI Design of prostaglandins with high binding affinity and selectivity for an IP2 receptor in the central nervous system and their biological activity
AU Suzuki, Masaaki; Kato, Koichi; Noyori, Ryoji; Watanabe, Yumiko; Sato, Takumi; Matsumura, Kiyoshi; Watanabe, Yasuyoshi
CS Faculty of Engineering, Gifu University, Japan
SO Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1998), 40th, 145-150
CODEN: TYKYDS
PB Nippon Kagakkai
DT Journal
LA Japanese
GI

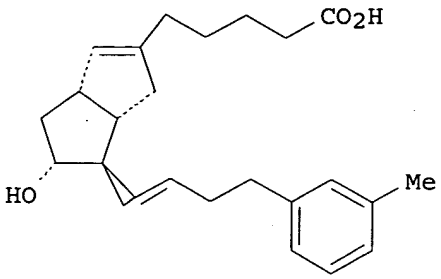
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The role of prostacyclin (PGI2) in the central nervous system (CNS) has still been unclear because of the lack of a specific ligand for a PGI2 receptor in CNS. In this context, the authors recently elaborated 15R-TIC (I; R = OH, R1 = H) with high binding affinity and selectivity for novel IP2 receptor which is specifically expressed in CNS neurons. The R configuration of the hydroxy-bearing C(15) in 15R-TIC is fascinating, because, in general, the configuration of biol. active PGs at C(15) position is known to be S. In this symposium, the authors describe synthesis of the TIC derivs. for structure-binding affinity relationship in addn. to biol. actions. 15-Deoxy-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (I; R = R1 = H) (referred to as 15-deoxy-TIC) exhibited, among others, highest binding affinity and selectivity for a IP2 receptor. I (R = R1 = H) has been prepd. based on the combination of the Witting reaction and Pd(0)-mediated coupling of an allyl carbonate and a sulfone. Thus, Witting reaction of aldehyde II (R2 = CHO, R3 = THP) and a Ph3P:CHCHO led to II [R2 = (E)-CH:CHCHO, R3 = THP]. The redn. of this followed by methoxycarbonylation gave allyl carbonate II [R2 = (E)-CH:CHCH2-OCO2Me, R3 = THP] which was treated with disulfone III in the presence of a 1:1 mixt. of Pd(0) and diphenylphosphinoethane to give II [R2 = (E)-CH:CHCH2-C(SO2Ph)2C6H4Me-m, R3 = THP]. Reductive removal of Ph sulfonyl groups of this and subsequent deprotection gave II (R2 = CH2CH2C6H4Me-m, R3 = H), which was hydrolyzed to give I (R = R1 = H). I (R, R1 = OH, H; H, H) prevented apoptotic cell death of hippocampal neurons induced under high oxygen (50%) atm., whereas I (R = H, R1 = OH), isocarbacyclin, and natural PGs except for PGI2 did not show such a biol. effect.

REFERENCE 3

AN 130:325022 CA

TI 15-Deoxy-16-(m-tolyl)-17,18,19,20-tetranorisocarbacyclin: a simple TIC derivative with potent anti-apoptotic activity for neuronal cells
AU Suzuki, Masaaki; Kato, Koichi; Noyori, Ryoji; Watanabe, Yumiko; Satoh, Takumi; Matsumura, Kiyoshi; Watanabe, Yasuyoshi
CS Faculty of Engineering, Department of Biomolecular Science, Gifu University, Gifu, 501-1193, Japan
SO Chemical Communications (Cambridge) (1999), (4), 307-308
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
GI



I

AB Biol. remarkable 15-deoxy-TIC (I) has been realized by the removal of the C(15) chiral center in 15R-TIC, a stable ligand for a CNS-type prostacyclin receptor (IP2); this deoxy deriv. exhibits ten-fold higher affinity and selectivity than 15R-TIC for the IP2 receptor in correlation with the anti-apoptotic activity for neuronal cells.
RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 4

AN 124:260630 CA
TI (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin: A stable ligand with high binding affinity and selectivity for a prostacyclin receptor in the central nervous system
AU Suzuki, Masaaki; Kato, Koichi; Noyori, Ryoji; Watanabe, Yumiko; Takechi, Hajime; Matsumura, Kiyoshi; Langstroem, Bengt; Watanabe, Yasuyoshi
CS Dep. Applied Chemistry, Gifu Univ., Gifu, 501-11, Japan
SO Angewandte Chemie, International Edition in English (1996), 35(3), 334-36
CODEN: ACIEAY; ISSN: 0570-0833
PB VCH
DT Journal
LA English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

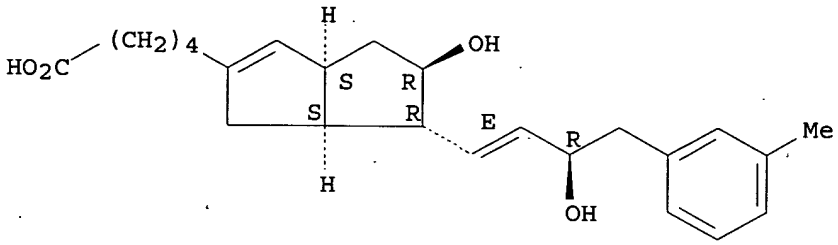
AB The title compd. I was devised based on the the structural modification of the .omega. side chain of isocarbacyclin (II), a chem. stable PGI2 agonist, starting from the aldehyde intermediate III.

L2 ANSWER 40 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 175169-68-3 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E,3R)-3-hydroxy-4-(3-methylphenyl)-1-butenyl]-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-

4-(3-methylphenyl)-1-butenyl]-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]-

OTHER NAMES:
CN (15R)-TIC
FS STEREOSEARCH
MF C24 H32 O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

12 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
12 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 138:384882 CA
TI Asymmetric catalysis: Science and opportunities (nobel lecture 2001)
AU Noyori, Ryoji
CS Department of Chemistry, Nagoya University, Nagoya, 464-8602, Japan
SO Advanced Synthesis & Catalysis (2003), 345(1+2), 15-32
CODEN: ASCAF7; ISSN: 1615-4150
PB Wiley-VCH Verlag GmbH & Co.' KGaA
DT Journal; General Review
LA English
AB A review on asym. catalysis as essential component of mol. science and technol. in the 21st century.is presented. The recent exceptional advances in this area attest to a range of conceptual breakthroughs in chem. sciences in general, and to the practical benefits of org. synthesis, not only in labs. but also in industry. Asym. catalysis by chiral organometallic complexes, early asym. hydrogenation, development of 2,2'-bis(diphenylphosphanyl)-1,1'-binaphthyl BINAP, asym. hydrogenation of olefins catalyzed by BINAP-Ruthenium complexes and of simple ketones by BINAP/diamine-ruthenium complexes, and asym. synthesis of menthol are discussed. Phenylbutenylpentalenepentanoic acid, (15R)-TIC, a selective prostaglandin (PG) PGI2-type carboxylic acid, obtained via asym. methodol. was found to show strong selective binding in the central nervous system, which thereby identifies the novel IP2 receptor.
RE.CNT 183 THERE ARE 183 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

AN 135:354710 CA
TI Creation of higher order prostaglandin (PG) probe for analysis of human brain function by positron emission tomography (PET)
AU Suzuki, Masaaki; Doi, Hisashi; Kato, Koichi
CS Fac. Eng., Gifu Univ., Japan
SO Farumashia (2001), 37(11), 994-998
CODEN: FARUAW; ISSN: 0014-8601
PB Pharmaceutical Society of Japan
DT Journal; General Review
LA Japanese

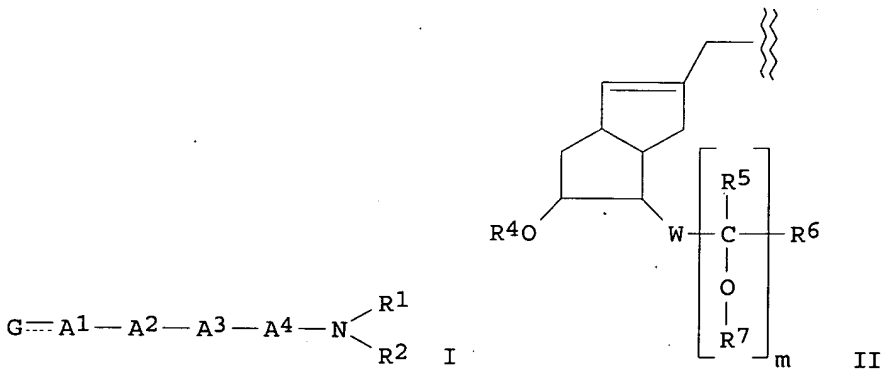
AB A review with refs., on development of a stable biochem. probes for study of functional roles of prostaglandin (PGI2) in the brain, discovery of a novel central type of PGI2 receptor (IP2) and prepn. of specific ligand (15R-TIC), neuroprotective activity of 15R-TIC, in vivo mol. imaging by PET, and prepn. of PET probes for imaging of brain IP2 receptor in humans and monkey.

REFERENCE 3

AN 134:173045 CA
TI Neuropathy improvers containing nitrogenous compounds as the active ingredient
IN Sugiura, Satoshi; Tsutsumi, Takaharu; Suwa, Yorimasa; Arai, Takami; Sakurai, Katsutoshi; Yoshioka, Noboru; Tanokura, Akira; Suzuki, Jun
PA Teijin Limited, Japan
SO PCT Int. Appl., 429 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001010433	A1	20010215	WO 2000-JP5287	20000807
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1201235	A1	20020502	EP 2000-950027	20000807
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	BR 2000012907	A	20020611	BR 2000-12907	20000807
PRAI	JP 1999-222259	19990805			
	JP 1999-222260	19990805			
	WO 2000-JP5287	20000807			

GI



AB Compds. represented by general formula (I); and neuropathy improvers contg. the same as the active ingredient: wherein G is a group represented by the general formula (II) or the like: [wherein R4 is hydrogen, acyl, or the like; W is a single bond, alkylene, or the like; m is 0 or 1; R5 and R6 are each hydrogen, an aliph. hydrocarbon group, an alicyclic hydrocarbon group, an arom. hydrocarbon group, a heterocyclic group, or the like; and R7 is hydrogen, acyl, alkoxycarbonyl, or the like]; A2 is a single bond, -O-, -NR3-, or -S(=O)n-; A1 and A3 are each a single bond, an aliph. hydrocarbon group, an alicyclic hydrocarbon group, a heterocyclic

group, phenylene, or the like; A4 is a single bond, carbonyl, an aliph. hydrocarbon group, or the like; and R1 and R2 are each hydrogen, alkyl, cycloalkyl, Ph, a heterocyclic group, or the like, these groups being each optionally substituted.

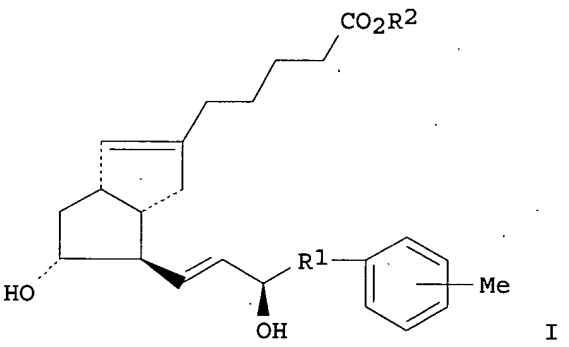
RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 4

AN 134:157581 CA
TI Neuropathy remedies
IN Suwa, Yorimasa; Yoshioka, Noboru; Arai, Takami; Sakurai, Katsutoshi; Suzuki, Jun; Watanabe, Yasuyoshi; Suzuki, Masaaki; Satoh, Takumi; Watanabe, Yumiko; Kataoka, Yosuke
PA Teijin Ltd., Japan; Osaka Bioscience Institute
SO PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001010445	A1	20010215	WO 2000-JP5267	20000804
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1208841	A1	20020529	EP 2000-950011	20000804
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				

PRAI JP 1999-222311 19990805
WO 2000-JP5267 20000804
GI



I

AB Remedies for nerve degeneration diseases contg. as the active ingredient (15R)-isocarbacyclin derivs. of general formula [I] or 15-deoxyisocarbacyclin derivs. In formula I, R1 is C1-C6 alkylene; and R2 is hydrogen, C1-C7 alkyl, or a protective group.

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 5

AN 133:99605 CA
TI Molecular Design of Prostaglandin Probes in Brain Research: High, Specific Binding to a Novel Prostacyclin Receptor in the Central Nervous System
AU Suzuki, Masaaki; Noyori, Ryoji; Langstrom, Bengt; Watanabe, Yasuyoshi
CS Dep. Biomol. Sci., Fac. Eng., Gifu University, Gifu, 501-1193, Japan

SO Bulletin of the Chemical Society of Japan (2000), 73(5), 1053-1070
CODEN: BCSJA8; ISSN: 0009-2673
PB Chemical Society of Japan
DT Journal; General Review
LA English
AB A review, with 56 refs. Mol. design to develop a stable biochem. probe for a study of the role of prostacyclin (PGI2) in the brain led to the discovery of (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacylin (referred to as 15R-TIC), that selectively bind to a novel PGI2 receptor, IP2, expressed in the central nervous system (CNS). This artificial prostaglandin with the 15R configuration exhibits high binding affinity for the IP2 receptor in the thalamus (IC50 = 32 nM) and weak affinity for the peripheral-type PGI2 receptor, IP1, in the NTS (IC50 = 1.2 .mu.M). The length of the .omega. side-chain and the position of the Me substituent on the arom. ring strongly influence the binding characteristics. The features of the IP2 receptor were elucidated by quant. mapping, specificity studies, and Scatchard anal., as well as by a study using knockout mice with a tritium-labeled 15R-TIC and related radioligands. In order to conduct in vivo PET studies, a rapid methylation reaction using Me iodide and an excess amt. of an aryltributylstannane has been developed. This has successfully been applied to the synthesis of short-lived 11C-incorporated PET tracers, 15R-[11C]TIC and its Me ester. The PET expts. accomplished the imaging of the IP2 receptor in the brain of living rhesus monkeys through i.v. administration. The elimination of the C(15) chirality results in 15-deoxy-TIC with ten-fold higher affinity and selectivity for the IP2 receptor than original 15R-TIC. Neither 15R-TIC nor 15-deoxy-TIC inhibit platelets aggregation, up to 400 nM, while PGI2 derivs. which bind with the IP1 receptor show a very potent inhibitory effect at a several nM level. Notably, these artificial CNS-specific PGI2 ligands, like the unstable natural PGI2 itself, prevent the apoptotic cell death of hippocampal neurons induced under high (50%) oxygen atm. and by xanthine and xanthine oxidase or serum deprivation. The difference in the binding potency between 15R-TIC and 15-deoxy-TIC for the IP2 receptor correlates well with the extent of the prevention of the neuronal cell death (IC50 values of 300 and 30 nM, resp., under high oxygen atm.). 15R-TIC protects CA1 pyramidal neurons against ischemic damage in gerbils. Thus, the designed TICs have neuronal survival-promoting activity both in vitro and in vivo, providing the possibility as a new type of chemotherapeutic agents for applications in neurodegeneration.
RE.CNT 108 THERE ARE 108 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 6

AN 132:45351 CA
TI Protective effect of prostaglandin I2 analogs on ischemic delayed neuronal damage in gerbils
AU Cui, Yilong; Kataoka, Yosky; Satoh, Takumi; Yamagata, Aya; Shirakawa, Noriyuki; Watanabe, Yumiko; Suzuki, Masaaki; Yanase, Hisato; Kataoka, Kiyoshi; Watanabe, Yasuyoshi
CS Department of Neuroscience, Osaka Bioscience Institute, Suita-shi, Osaka, 565-0874, Japan
SO Biochemical and Biophysical Research Communications (1999), 265(2), 301-304
CODEN: BBRCA9; ISSN: 0006-291X
PB Academic Press
DT Journal
LA English
AB The authors found a novel subtype of prostaglandin (PG) I2 receptor (IP2) expressed in the central nervous system. Recently the authors have demonstrated that (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (15R-TIC) and 15-deoxy-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (15-deoxy-TIC), IP2-specific ligands, significantly prevented high (50%) oxygen-induced apoptotic neuronal death in cultured hippocampal neurons. The authors report a potent neuroprotective effect of such analogs on delayed neuronal death of hippocampal CA1 neurons following transient ischemia for 3 min in gerbils. (15S)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (15S-TIC), which nonselectively acts both on the

PGI2 receptor expressed in the peripheral tissue (IP1) and on IP2, also showed a neuroprotective effect on such an ischemic model at higher doses than those for 15R-TIC and 15-deoxy-TIC. These PGI2 analogs did not affect brain temp., indicating that the agents showed the neuroprotective effect not by a hypothermic effect, but rather by the direct action on neurons. (c) 1999 Academic Press.

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 7

AN 131:139854 CA
TI A novel subtype of prostacyclin receptor in the central nervous system
AU Watanabe, Yumiko; Matsumura, Kiyoshi; Takechi, Hajime; Kato, Koichi; Morii, Hiroshi; Bjorkman, Margareta; Langstrom, Bengt; Noyori, Ryoji; Suzuki, Masaaki; Watanabe, Yasuyoshi
CS Subfemtomole Biorecognition Project, ICORP, Department of Neuroscience, Osaka Bioscience Institute, Japan Science and Technology Corporation, Osaka, 565-0874, Japan
SO Journal of Neurochemistry (1999), 72(6), 2583-2592
CODEN: JONRA9; ISSN: 0022-3042
PB Lippincott Williams & Wilkins
DT Journal
LA English
AB Recently, in the course of the authors' search for the prostacyclin receptor in the brain, the authors found a novel subtype, designated as IP2, which was finely discriminated by use of the specific ligand (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (15R-TIC) and specifically localized in the rostral part of the brain. In the present study, the tritiated compd. 15R-[15-3H]TIC was synthesized and utilized for more specific research on IP2. The specificity of binding to rat brain regions was confirmed by use of several prostacyclin derivs. including 15S-TIC. Mapping of 15R- and 15S-[3H]TIC binding in adjacent pairs of frozen sections of rat brain demonstrated a quite similar pattern of distribution in almost all rostral brain regions, indicating that the regions may contain only the IP2 subtype. 15R-[3H]TIC binding was very faint as compared with 15S-[3H]TIC binding in the caudal medullary region. High densities of 15R-[3H]TIC binding sites were shown in the dorsal part of the lateral septal nucleus, thalamic nuclei, limbic structures, and some of the cortical regions. Scatchard plot anal. showed two components of high-affinity 15R-[3H]TIC binding in the rostral regions, one with a KD value at .apprx.1 nM and the other with .apprx.30 nM. These results strengthen the authors' previous finding that a different subtype of prostacyclin receptor is expressed in the CNS, and the map with 15R-[3H]TIC obtained here could guide further studies on the mol. and functional properties of the IP2.

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 8

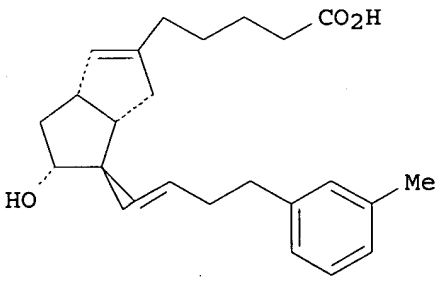
AN 131:129774 CA
TI Design of prostaglandins with high binding affinity and selectivity for an IP2 receptor in the central nervous system and their biological activity
AU Suzuki, Masaaki; Kato, Koichi; Noyori, Ryoji; Watanabe, Yumiko; Sato, Takumi; Matsumura, Kiyoshi; Watanabe, Yasuyoshi
CS Faculty of Engineering, Gifu University, Japan
SO Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1998), 40th, 145-150
CODEN: TYKYDS
PB Nippon Kagakkai
DT Journal
LA Japanese
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The role of prostacyclin (PGI2) in the central nervous system (CNS) has still been unclear because of the lack of a specific ligand for a PGI2 receptor in CNS. In this context, the authors recently elaborated 15R-TIC (I; R = OH, R1 = H) with high binding affinity and selectivity for novel IP2 receptor which is specifically expressed in CNS neurons. The R configuration of the hydroxy-bearing C(15) in 15R-TIC is fascinating, because, in general, the configuration of biol. active PGs at C(15) position is known to be S. In this symposium, the authors describe synthesis of the TIC derivs. for structure-binding affinity relationship in addn. to biol. actions. 15-Deoxy-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin (I; R = R1 = H) (referred to as 15-deoxy-TIC) exhibited, among others, highest binding affinity and selectivity for a IP2 receptor. I (R = R1 = H) has been prepd. based on the combination of the Witting reaction and Pd(0)-mediated coupling of an allyl carbonate and a sulfone. Thus, Witting reaction of aldehyde II (R2 = CHO, R3 = THP) and a Ph3P:CHCHO led to II [R2 = (E)-CH:CHCHO, R3 = THP]. The redn. of this followed by methoxycarbonylation gave allyl carbonate II [R2 = (E)-CH:CHCH2-OCO2Me, R3 = THP] which was treated with disulfone III in the presence of a 1:1 mixt. of Pd(0) and diphenylphosphinoethane to give II [R2 = (E)-CH:CHCH2-C(SO2Ph)2C6H4Me-m, R3 = THP]. Reductive removal of Ph sulfonyl groups of this and subsequent deprotection gave II (R2 = CH2CH2C6H4Me-m, R3 = H), which was hydrolyzed to give I (R = R1 = H). I (R, R1 = OH, H; H, H) prevented apoptotic cell death of hippocampal neurons induced under high oxygen (50%) atm., whereas I (R = H, R1 = OH), isocarbacyclin, and natural PGs except for PGI2 did not show such a biol. effect.

REFERENCE 9

AN 130:325022 CA
TI 15-Deoxy-16-(m-tolyl)-17,18,19,20-tetranorisocarbacyclin: a simple TIC derivative with potent anti-apoptotic activity for neuronal cells
AU Suzuki, Masaaki; Kato, Koichi; Noyori, Ryoji; Watanabe, Yumiko; Satoh, Takumi; Matsumura, Kiyoshi; Watanabe, Yasuyoshi
CS Faculty of Engineering, Department of Biomolecular Science, Gifu University, Gifu, 501-1193, Japan
SO Chemical Communications (Cambridge) (1999), (4), 307-308
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
GI



I

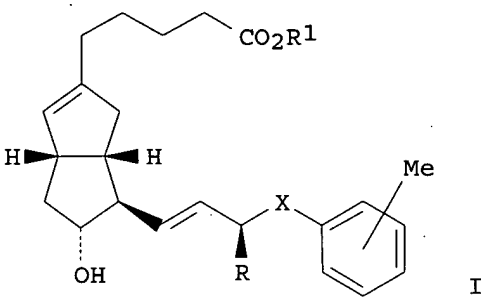
AB Biol. remarkable 15-deoxy-TIC (I) has been realized by the removal of the C(15) chiral center in 15R-TIC, a stable ligand for a CNS-type prostacyclin receptor (IP2); this deoxy deriv. exhibits ten-fold higher affinity and selectivity than 15R-TIC for the IP2 receptor in correlation with the anti-apoptotic activity for neuronal cells.
RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 10

AN 130:311654 CA
TI Preparation of a (15R)-isocarbacyclin or 15-deoxy-isocarbacyclin derivatives for use as neuron apoptosis inhibitors
IN Watanabe, Yasuyoshi; Suzuki, Masaaki; Watanabe, Yumiko; Hazato, Atsuo; Sato, Takumi
PA Japan Science and Technology Corporation, Japan
SO Eur. Pat. Appl., 16 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 911314	A1	19990428	EP 1998-308570	19981020
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	US 6087395	A	20000711	US 1998-173758	19981016
	CA 2251241	AA	19990421	CA 1998-2251241	19981020
	CN 1219389	A	19990616	CN 1998-120984	19981020
	JP 11222436	A2	19990817	JP 1998-300151	19981021
PRAI	JP 1997-288912		19971021		

GI



I

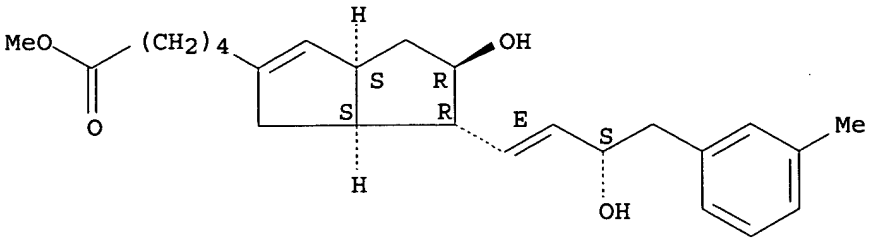
AB An efficient and low cost prepn. of isocarbacyclin derivs. I [R = H, OH; R1 = H, carboxy protecting group; X = 1-6 carbon chain] for pharmaceutical use as neuron apoptosis inhibitors was described. Thus, 15-deoxy-isocarbacyclin 3-tolyl deriv. I (R = R1 = H, X = CH2) was prepd. starting from (3aS,5R,6R,6aS)-6-formyl-1,3a,4,5,6,6a-hexahydro-5-[(tetrahydro-2H-pyran-2-yl)oxy]-2-pentalenepentanoic acid Me ester, (triphenylphosphoranylidine)acetaldehyde and 1-[bis(phenylsulfonyl)methyl]-3-methylbenzene. The prepd. compds. were tested for neuron apoptosis inhibiting activity on hippocampal CA1 pyramidal neurons apoptosis in Mongolian gerbils.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 41 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 175169-67-2 REGISTRY
CN 2-Pentalenepentanoic acid, 3,3a,4,5,6,6a-hexahydro-5-hydroxy-4-[(1E,3S)-3-hydroxy-4-(3-methylphenyl)-1-butenyl]-, methyl ester, (3aS,4R,5R,6aS)-(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-4-(3-methylphenyl)-1-butenyl]-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]-
OTHER NAMES:
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[(1E,3S)-3-hydroxy-4-(3-methylphenyl)-1-butenyl]-, methyl ester, (3aS,5R,6R,6aS)-
FS STEREOSEARCH
MF C25 H34 O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

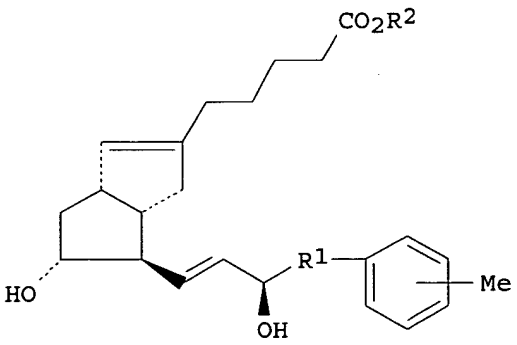
4 REFERENCES IN FILE CA (1957 TO DATE)
4 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 134:157581 CA
TI Neuropathy remedies
IN Suwa, Yorimasa; Yoshioka, Noboru; Arai, Takami; Sakurai, Katsutoshi; Suzuki, Jun; Watanabe, Yasuyoshi; Suzuki, Masaaki; Satoh, Takumi; Watanabe, Yumiko; Kataoka, Yosuke
PA Teijin Ltd., Japan; Osaka Bioscience Institute
SO PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001010445	A1	20010215	WO 2000-JP5267	20000804
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1208841	A1	20020529	EP 2000-950011	20000804
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
PRAI	JP 1999-222311		19990805		
	WO 2000-JP5267		20000804		

GI



I

AB Remedies for nerve degeneration diseases contg. as the active ingredient (15R)-isocarbacyclin derivs. of general formula [I] or

15-deoxyisocarbacyclin derivs. In formula I, R1 is C1-C6 alkylene; and R2 is hydrogen, C1-C7 alkyl, or a protective group.
RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

AN 134:41988 CA
TI Rapid Methylation for the Synthesis of a 11C-Labeled Tolylisocarbacyclin Imaging the IP2 Receptor in a Living Human Brain
AU Suzuki, M.; Doi, H.; Kato, K.; Bjorkman, M.; Langstrom, B.; Watanabe, Y.; Noyori, R.
CS Faculty of Engineering, Department of Biomolecular Science, Gifu University, Gifu, 501-1193, Japan
SO Tetrahedron (2000), 56(42), 8263-8273
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier Science Ltd.
DT Journal
LA English
AB A rapid method for Pd-promoted cross-coupling of Me iodide and tributyltin derivs. of tolylisocarbacyclins was developed with the objective of applying to the PET study on the IP2 receptor in a living human brain. The high efficiency is obtainable for both of the one-pot operation using a large excess of CuCl and the stepwise operation consisting of the initial prepn. of a methylpalladium complex followed by mixing with the remaining requisite materials for the cross-coupling. The latter protocol allowed for the highly reproducible synthesis of an actual PET tracer with total radioactivity of several GBq. Several stannanes could be employed as precursors of PET tracers in this rapid cross-coupling reaction.
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 3

AN 126:59803 CA
TI Isocarbacyclin derivatives
IN Watanabe, Yasuyoshi; Suzuki, Masaaki; Hazato, Atsuo; Langstrom, Bengt
PA Research Development Corporation of Japan, Japan
SO Can. Pat. Appl., 39 pp.
CODEN: CPXXEB
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 2168514	AA	19960911	CA 1996-2168514	19960131
	JP 08245498	A2	19960924	JP 1995-51589	19950310
	JP 3250936	B2	20020128		
	JP 2002128730	A2	20020509	JP 2001-250732	19950310
	US 5700833	A	19971223	US 1996-594152	19960131
PRAI	JP 1995-51589		19950310		

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention provides novel isocarbacyclin derivs. I [R = H, alkyl, cation; X = alkylene] useful for search and study of the prostacyclin receptor and as a therapeutic drug for central nervous system diseases. Thus, 13,14-dihydroxy-13,14-dihydroisocarbacyclin Me ester was oxidized with NaIO4 and treated with 3-MeC6H4CH2COCH2P(O)(OMe)2, followed by redn. and ester hydrolysis to give the acid II. II bound to both thalamic and medulla oblongata nuclear prostacyclin receptors but showed no platelet aggregation inhibiting activity.

REFERENCE 4

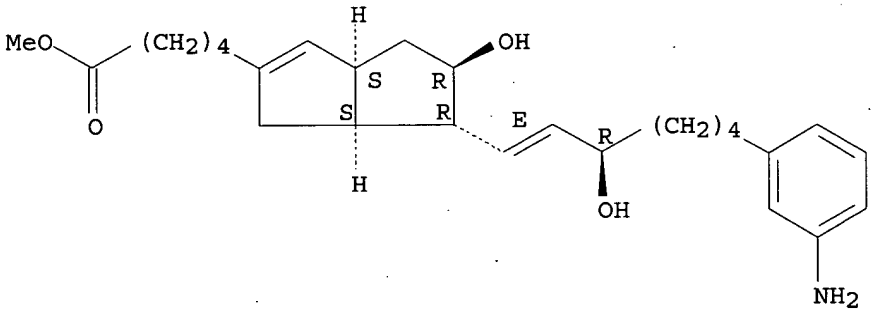
AN 124:260630 CA
TI (15R)-16-m-tolyl-17,18,19,20-tetranorisocarbacyclin: A stable ligand with high binding affinity and selectivity for a prostacyclin receptor in the central nervous system
AU Suzuki, Masaaki; Kato, Koichi; Noyori, Ryoji; Watanabe, Yumiko; Takechi, Hajime; Matsumura, Kiyoshi; Langstroem, Bengt; Watanabe, Yasuyoshi
CS Dep. Applied Chemistry, Gifu Univ., Gifu, 501-11, Japan
SO Angewandte Chemie, International Edition in English (1996), 35(3), 334-36
CODEN: ACIEAY; ISSN: 0570-0833
PB VCH
DT Journal
LA English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compd. I was devised based on the the structural modification of the .omega. side chain of isocarbacyclin (II), a chem. stable PGI2 agonist, starting from the aldehyde intermediate III.

L2 ANSWER 42 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 153060-02-7 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[7-(3-aminophenyl)-3-hydroxy-1-heptenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H39 N O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 120:134138 CA
TI Preparation of isocarbacylin derivatives as prostacyclin-like drugs and agents for photoaffinity labeling of proteins
IN Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Negishi, Manabu; Hashimoto, Hitoshi; Ichikawa, Atsushi; Ito, Seiji
PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1
PATENT NO. KIND DATE APPLICATION NO. DATE

PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175	19911218			

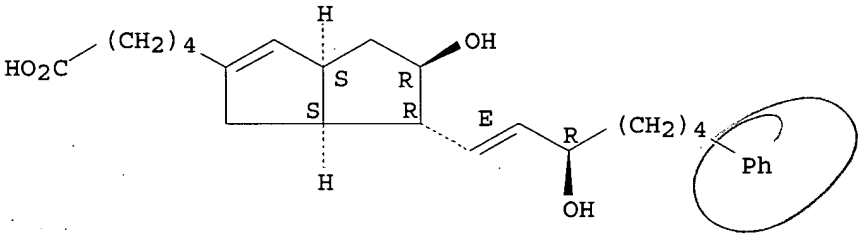
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [R1 = H, alkyl; X = H, tritium; Y = H, azido, (trityl)amino; n = 1 - 7] were prepd. Redn. of isocarbacyclin II with [3H]-NaBH4-CeCl3.7H2O (60 Ci/mmol), followed by sapon. and workup, gave isocarbacyclin III. Photoaffinity labeling of PGI2 receptor protein using III indicated that the mol. wt. of the said protein was 43K. Several I showed affinity for prostacyclin receptors.

L2 ANSWER 43 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 153060-01-6 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-(3-hydroxy-7-phenyl-1-heptenyl)-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H36 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 120:134138 CA
TI Preparation of isocarbacylin derivatives as prostacyclin-like drugs and agents for photoaffinity labeling of proteins
IN Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Negishi, Manabu; Hashimoto, Hitoshi; Ichikawa, Atsushi; Ito, Seiji
PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175	19911218			

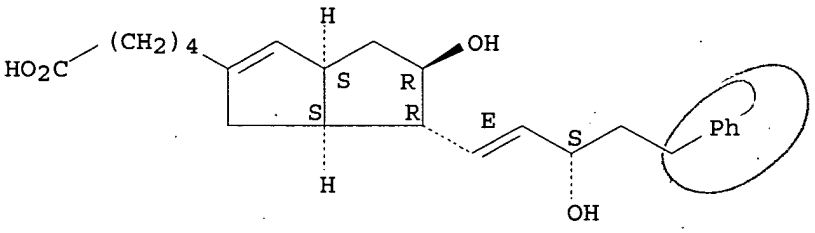
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [R1 = H, alkyl; X = H, tritium; Y = H, azido, (trityl)amino; n = 1 - 7] were prepd. Redn. of isocarbacyclin II with [3H]-NaBH4-CeCl3.7H2O (60 Ci/mmol), followed by sapon. and workup, gave isocarbacyclin III. Photoaffinity labeling of PGI2 receptor protein using III indicated that the mol. wt. of the said protein was 43K. Several I showed affinity for prostacyclin receptors.

L2 ANSWER 44 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 153060-00-5 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-(3-hydroxy-5-phenyl-1-pentenyl)-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H32 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 120:134138 CA
TI Preparation of isocarbacylin derivatives as prostacyclin-like drugs and agents for photoaffinity labeling of proteins
IN Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Negishi, Manabu; Hashimoto, Hitoshi; Ichikawa, Atsushi; Ito, Seiji .
PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

GI

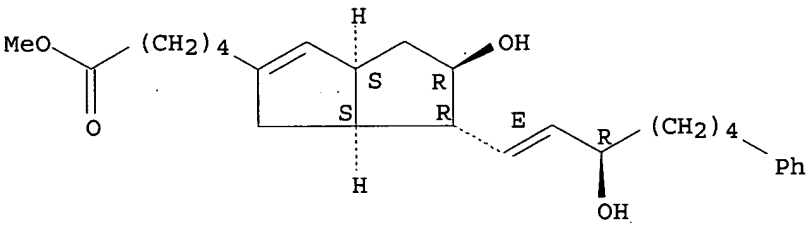
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [R1 = H, alkyl; X = H, tritium; Y = H, azido, (trityl)amino; n = 1 - 7] were prepd. Redn. of isocarbacyclin II with [3H]-NaBH4-CeCl3.7H2O (60 Ci/mmol), followed by sapon. and workup, gave isocarbacyclin III. Photoaffinity labeling of PGI2 receptor protein using III indicated that the mol. wt. of the said protein was 43K. Several I

showed affinity for prostacyclin receptors.

L2 ANSWER 45 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 153059-99-5 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-(3-hydroxy-7-phenyl-1-heptenyl)-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H38 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 120:134138 CA
TI Preparation of isocarbacylin derivatives as prostacyclin-like drugs and agents for photoaffinity labeling of proteins
IN Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Negishi, Manabu; Hashimoto, Hitoshi; Ichikawa, Atsushi; Ito, Seiji
PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

GI

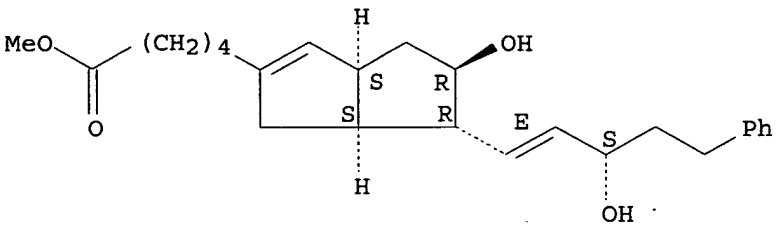
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [R1 = H, alkyl; X = H, tritium; Y = H, azido, (trityl)amino; n = 1 - 7] were prepd. Redn. of isocarbacyclin II with [3H]-NaBH4-CeCl3.7H2O (60 Ci/mmol), followed by sapon. and workup, gave isocarbacyclin III. Photoaffinity labeling of PGI2 receptor protein using III indicated that the mol. wt. of the said protein was 43K. Several I showed affinity for prostacyclin receptors.

L2 ANSWER 46 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 153059-98-4 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-(3-hydroxy-5-phenyl-1-pentenyl)-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH

MF C25 H34 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 120:134138 CA
TI Preparation of isocarbacylin derivatives as prostacyclin-like drugs and agents for photoaffinity labeling of proteins
IN Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Negishi, Manabu; Hashimoto, Hitoshi; Ichikawa, Atsushi; Ito, Seiji
PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

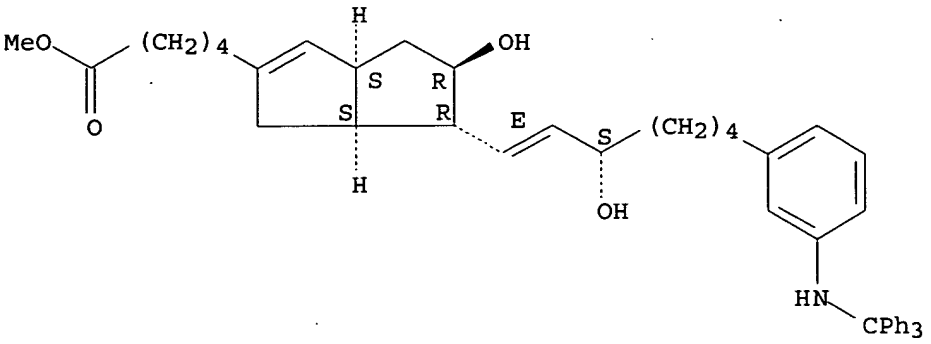
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [R1 = H, alkyl; X = H, tritium; Y = H, azido, (trityl)amino; n = 1 - 7] were prepd. Redn. of isocarbacyclin II with [3H]-NaBH4-CeCl3.7H2O (60 Ci/mmol), followed by sapon. and workup, gave isocarbacyclin III. Photoaffinity labeling of PGI2 receptor protein using III indicated that the mol. wt. of the said protein was 43K. Several I showed affinity for prostacyclin receptors.

L2 ANSWER 47 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 153059-97-3 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-7-[3-[(triphenylmethyl)amino]phenyl]-1-heptenyl]-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C46 H53 N O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 120:134138 CA
TI Preparation of isocarbacylin derivatives as prostacyclin-like drugs and agents for photoaffinity labeling of proteins
IN Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Negishi, Manabu; Hashimoto, Hitoshi; Ichikawa, Atsushi; Ito, Seiji
PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

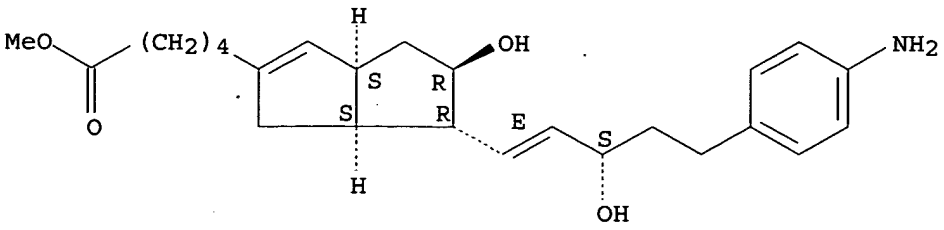
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [R1 = H, alkyl; X = H, tritium; Y = H, azido, (trityl)amino; n = 1 - 7] were prepd. Redn. of isocarbacyclin II with [3H]-NaBH4-CeCl3.7H2O (60 Ci/mmol), followed by sapon. and workup, gave isocarbacyclin III. Photoaffinity labeling of PGI2 receptor protein using III indicated that the mol. wt. of the said protein was 43K. Several I showed affinity for prostacyclin receptors.

L2 ANSWER 48 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 153059-96-2 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[5-(4-aminophenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H35 N O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 120:134138 CA
TI Preparation of isocarbacylin derivatives as prostacyclin-like drugs and agents for photoaffinity labeling of proteins
IN Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Negishi, Manabu; Hashimoto, Hitoshi; Ichikawa, Atsushi; Ito, Seiji
PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 05163194	A2	19930629	JP 1991-353175	19911218
JP 2872468	B2	19990317		
PRAI JP 1991-353175		19911218		

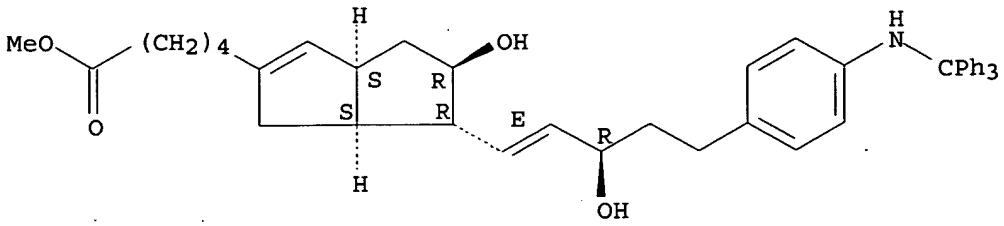
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [R1 = H, alkyl; X = H, tritium; Y = H, azido, (trityl)amino; n = 1 - 7] were prepd. Redn. of isocarbacyclin II with [3H]-NaBH4-CeCl3.7H2O (60 Ci/mmol), followed by sapon. and workup, gave isocarbacyclin III. Photoaffinity labeling of PGI2 receptor protein using III indicated that the mol. wt. of the said protein was 43K. Several I showed affinity for prostacyclin receptors.

L2 ANSWER 49 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 153059-95-1 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-5-[4-[(triphenylmethyl)amino]phenyl]-1-pentenyl]-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C44 H49 N O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



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1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

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PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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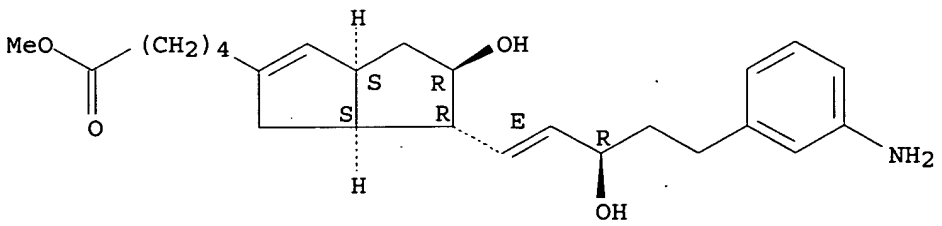
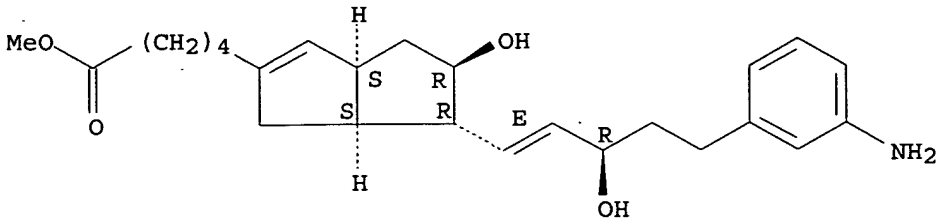
L2 ANSWER 50 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 153059-94-0 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[5-(3-aminophenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H35 N O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.





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SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

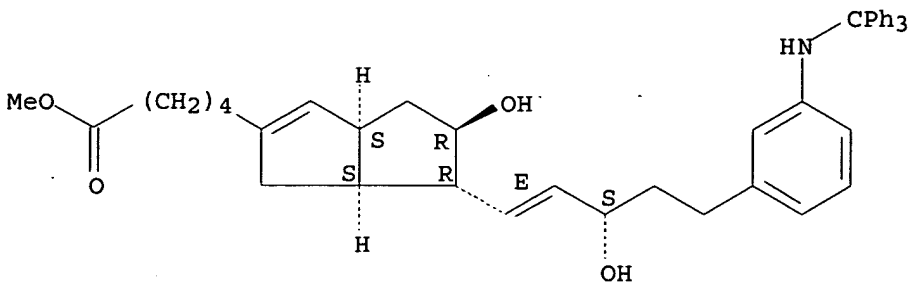
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [R1 = H, alkyl; X = H, tritium; Y = H, azido, (trityl)amino; n = 1 - 7] were prepd. Redn. of isocarbacyclin II with [3H]-NaBH4-CeCl3.7H2O (60 Ci/mmol), followed by sapon. and workup, gave isocarbacyclin III. Photoaffinity labeling of PGI2 receptor protein using III indicated that the mol. wt. of the said protein was 43K. Several I showed affinity for prostacyclin receptors.

L2 ANSWER 51 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 153059-93-9 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-5-[3-[(triphenylmethyl)amino]phenyl]-1-pentenyl]-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C44 H49 N O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



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SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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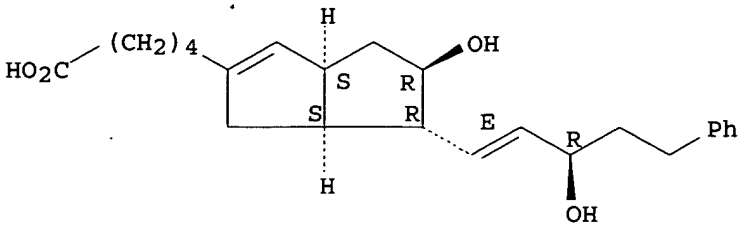
L2 ANSWER 52 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 152934-73-1 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-(3-hydroxy-5-phenyl-1-pentenyl)-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H32 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
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REFERENCE 1

AN 120:134138 CA
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PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05163194	A2	19930629	JP 1991-353175	19911218
JP 2872468	B2	19990317		

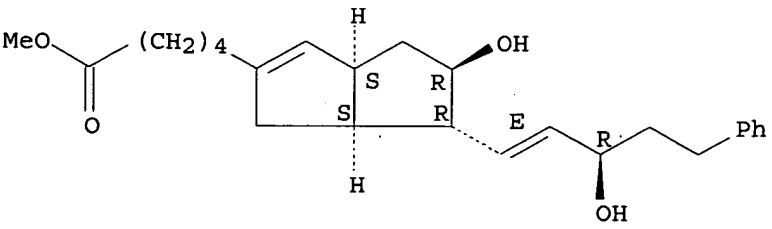
PRAI JP 1991-353175 19911218
GI

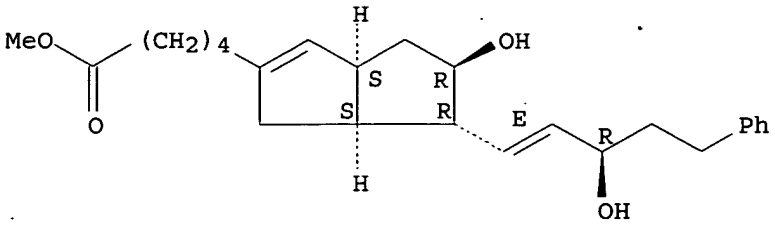
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [R1 = H, alkyl; X = H, tritium; Y = H, azido, (trityl)amino; n = 1 - 7] were prepd. Redn. of isocarbacyclin II with [3H]-NaBH4-CeCl3.7H2O (60 Ci/mmol), followed by sapon. and workup, gave isocarbacyclin III. Photoaffinity labeling of PGI2 receptor protein using III indicated that the mol. wt. of the said protein was 43K. Several I showed affinity for prostacyclin receptors.

L2 ANSWER 53 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 152934-71-9 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-(3-hydroxy-5-phenyl-1-pentenyl)-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H34 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.





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1 REFERENCES IN FILE CA (1957 TO DATE)
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SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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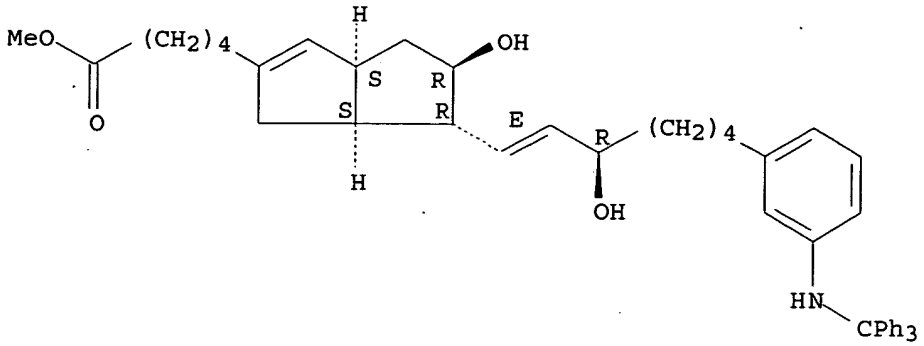
L2 ANSWER 54 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 152934-69-5 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-7-[3-[(triphenylmethyl)amino]phenyl]-1-heptenyl]-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C46 H53 N O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 120:134138 CA
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PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

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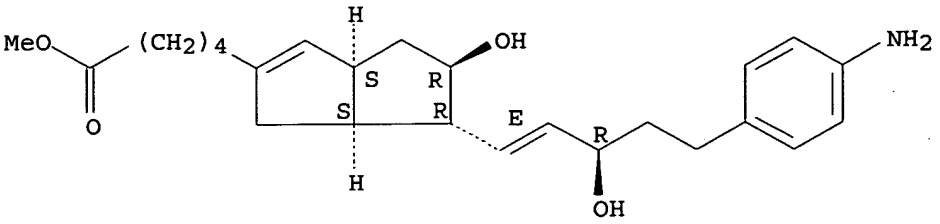
L2 ANSWER 55 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 152934-67-3 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[5-(4-aminophenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H35 N O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



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SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

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	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

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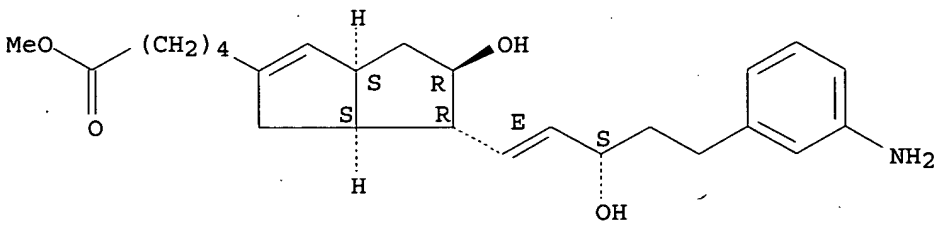
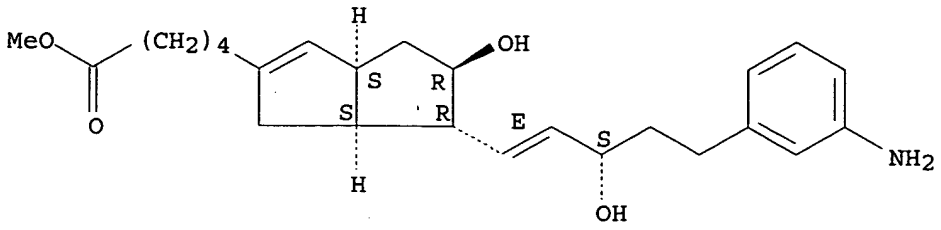
L2 ANSWER 56 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 152934-65-1 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[5-(3-aminophenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H35 N O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.





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CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

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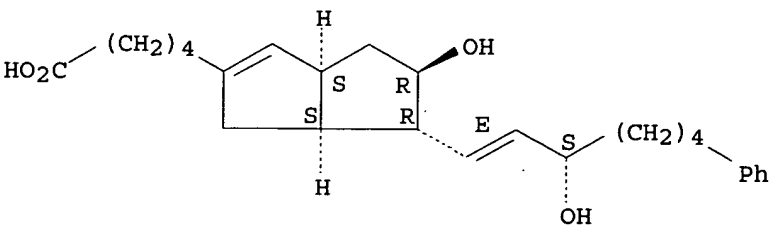
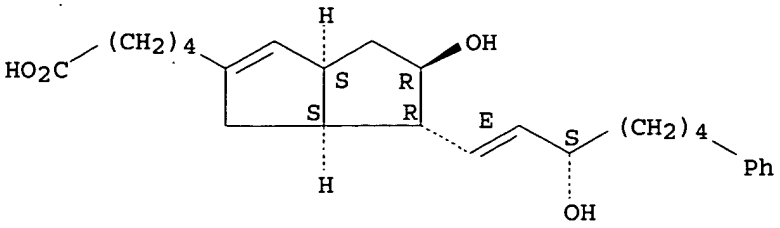
L2 ANSWER 57 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 152934-63-9 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-(3-hydroxy-7-phenyl-1-heptenyl)-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H36 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.





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PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

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	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

GI

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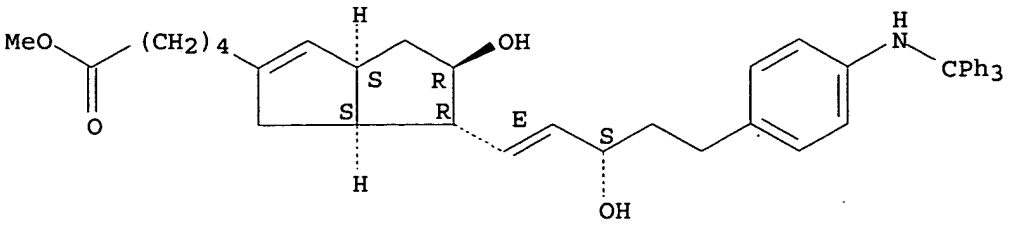
L2 ANSWER 58 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 152934-62-8 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-5-[4-[(triphenylmethyl)amino]phenyl]-1-pentenyl]-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C44 H49 N O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



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1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

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AN 120:134138 CA
TI Preparation of isocarbacylin derivatives as prostacyclin-like drugs and agents for photoaffinity labeling of proteins
IN Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Negishi, Manabu; Hashimoto, Hitoshi; Ichikawa, Atsushi; Ito, Seiji
PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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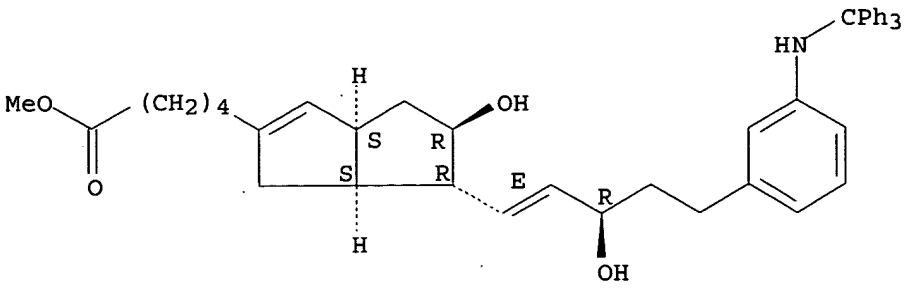
L2 ANSWER 59 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 152934-61-7 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-[3-hydroxy-5-[3-[(triphenylmethyl)amino]phenyl]-1-pentenyl]-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C44 H49 N O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 120:134138 CA
TI Preparation of isocarbacylin derivatives as prostacyclin-like drugs and agents for photoaffinity labeling of proteins
IN Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Negishi, Manabu; Hashimoto, Hitoshi; Ichikawa, Atsushi; Ito, Seiji
PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
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	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

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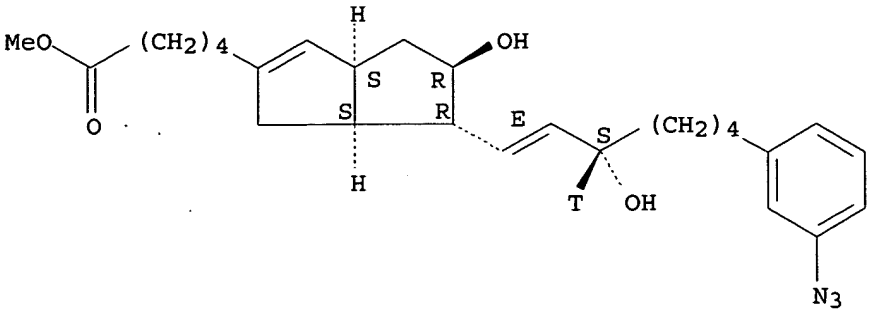
L2 ANSWER 60 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 141979-58-0 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[7-(3-azidophenyl)-3-hydroxy-1-heptenyl-3-t]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H36 N3 O4 T
SR CA
LC STN Files: CA, CAPLUS

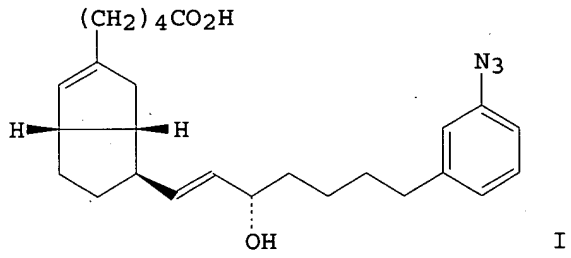
Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 117:26122 CA
TI An azido-functionalized isocarbacyclin analog acting as an efficient photoaffinity probe for a prostacyclin receptor
AU Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Hashimoto, Hitoshi; Negishi, Manabu; Ichikawa, Atsushi; Ito, Seiji
CS Chem. Instrum. Cent., Nagoya Univ., Chikusa, 464-01, Japan
SO Tetrahedron (1992), 48(13), 2635-58
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
GI

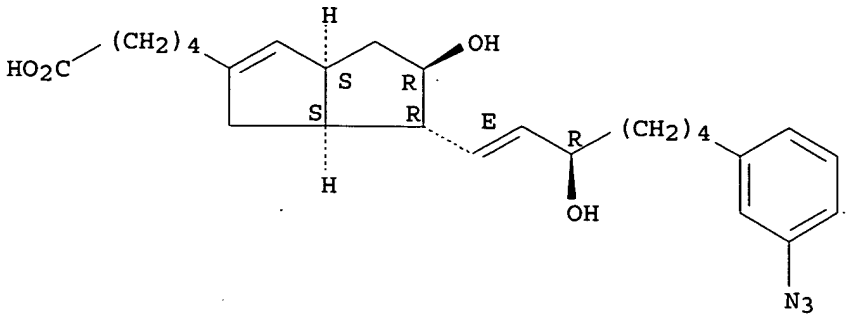


I

AB A stable prostacyclin analog, I, having an azidophenyl group as a photoaffinity labeling functionality has been synthesized. I has a sufficiently high affinity to the prostacyclin receptor protein in mastocytoma P-815 cells, exhibiting an IC50 value of 3 nM for the replacement of iloprost bound to the receptor protein. A photoaffinity probe compd., [3H]-I, is obtainable by redn. of the ketone with NaB3H4-CeCl3 followed by alk. hydrolysis of the Me ester.

L2 ANSWER 61 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 141978-78-1 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[7-(3-azidophenyl)-3-hydroxy-1-heptenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H35 N3 O4
SR CA
LC STN Files: CA, CAPLUS, CHEMINFORMRX

Absolute stereochemistry.
Double bond geometry as shown.



2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 120:134138 CA
TI Preparation of isocarbacylin derivatives as prostacyclin-like drugs and agents for photoaffinity labeling of proteins
IN Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Negishi, Manabu; Hashimoto, Hitoshi; Ichikawa, Atsushi; Ito, Seiji
PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05163194	A2	19930629	JP 1991-353175	19911218
JP 2872468	B2	19990317		

PRAI JP 1991-353175 19911218
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [R1 = H, alkyl; X = H, tritium; Y = H, azido, (trityl)amino; n = 1 - 7] were prepd. Redn. of isocarbacyclin II with [3H]-NaBH4-CeCl3.7H2O (60 Ci/mmol), followed by sapon. and workup, gave isocarbacyclin III. Photoaffinity labeling of PGI2 receptor protein using III indicated that the mol. wt. of the said protein was 43K. Several I showed affinity for prostacyclin receptors.

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AN 117:26122 CA
TI An azido-functionalized isocarbacyclin analog acting as an efficient photoaffinity probe for a prostacyclin receptor
AU Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Hashimoto, Hitoshi; Negishi, Manabu; Ichikawa, Atsushi; Ito, Seiji
CS Chem. Instrum. Cent., Nagoya Univ., Chikusa, 464-01, Japan
SO Tetrahedron (1992), 48(13), 2635-58
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
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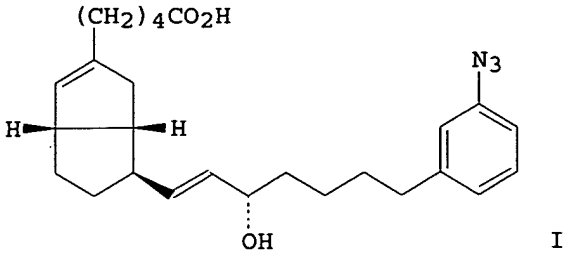

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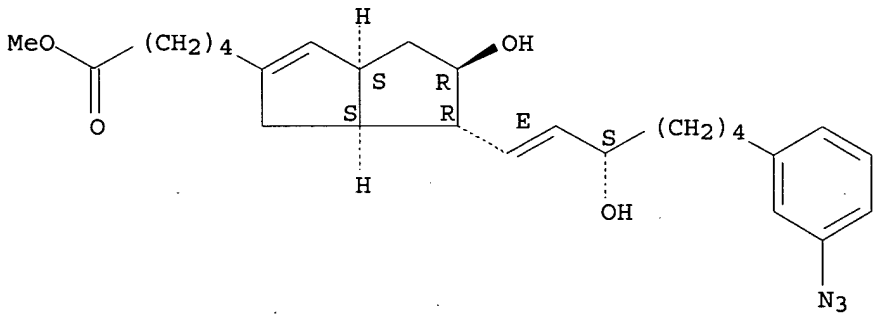
L2 ANSWER 62 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 141978-77-0 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[7-(3-azidophenyl)-3-hydroxy-1-heptenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H37 N3 O4
SR CA
LC STN Files: CA, CAPLUS, CHEMINFORMRX

Absolute stereochemistry.
Double bond geometry as shown.



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SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

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	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

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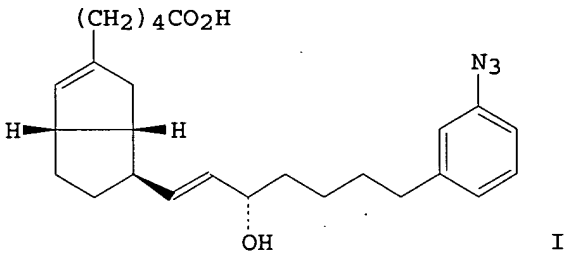

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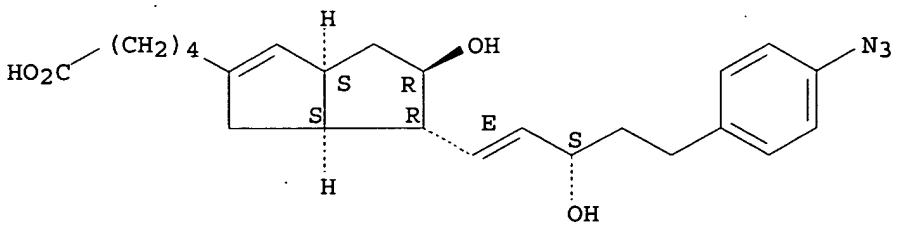
L2 ANSWER 63 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 141978-76-9 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[5-(4-azidophenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H31 N3 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



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SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 2872468	B2	19990317		

PRAI JP 1991-353175 19911218
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CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
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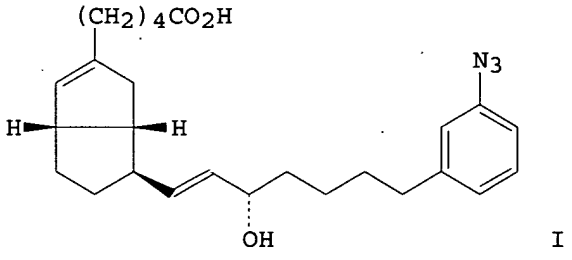

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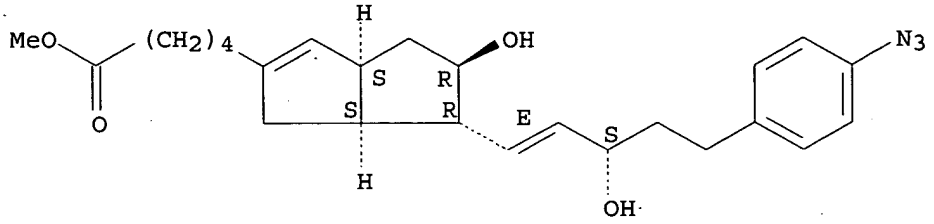
L2 ANSWER 64 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 141978-75-8 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[5-(4-azidophenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H33 N3 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



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CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

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	JP 2872468	B2	19990317		
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SO Tetrahedron (1992), 48(13), 2635-58
CODEN: TETRAB; ISSN: 0040-4020

DT Journal
LA English
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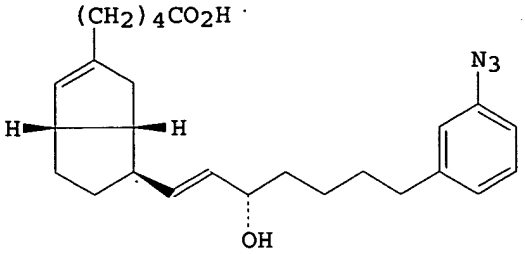

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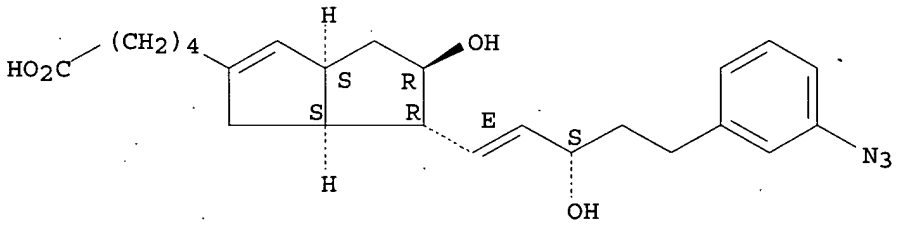
L2 ANSWER 65 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 141978-74-7 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[(1E,3S)-5-(3-azidophenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, (3aS,5R,6R,6aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pentalenepentanoic acid, 6-[5-(3-azidophenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]-
FS STEREOSEARCH
MF C24 H31 N3 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



3 REFERENCES IN FILE CA (1957 TO DATE)
3 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 129:4520 CA
TI Preparation of isocarbacyclin derivatives, their radiolabeled compounds, and their use as photoaffinity labeling probes
IN Watanabe, Yasuyoshi; Hasato, Atsuo; Watanabe, Yumiko; Suzuki, Masaki
PA Foundation for Scientific Technology Promotion, Japan; Hasato, Atsuo
SO Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI JP 10087608 A2 19980407 JP 1996-243122 19960913
PRAI JP 1996-243122 19960913
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The derivs. I (R1 = H, alkyl, cation; R2 = alkylene; R3 = H, Me) are prepd. by treatment of Horner-Emmons reagents II with formyl compds. III (R4 = C1-5 alkyl; R5 = H, tetrahydropyranyl) in the presence of bases, deprotection of OH-protective group if necessary, redn. of the resulting ketones IV, and hydrolysis if necessary. Also claimed are I labeled with 3H, 11C, or 14C at the arbitrary position and photoaffinity labeling using the radiolabeled I as probes, esp. for labeling of prostacyclin receptors. I are also useful as drugs for central nervous system disorders. A MeOH soln. of 16-(3-azidophenyl)-15-dehydro-17,18,19,20-tetranorisocarbacyclin Me ester prepd. from di-Me 2-oxo-3-(3-azidophenyl)propylphosphonate and III (R4 = Me, R5 = H), was treated with CeCl3.7H2O at room temp. then NaBH4 at 0.degree., and the resulting product was fractionated by silica gel chromatog. to give 48% 16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester and 49% 15-epi-16-(3-Azidophenyl)-17,18,19,20-tetranorisocarbacyclin Me ester (V). A MeOH soln. of V was treated with an aq. NaOH soln. to give 96% free acid (VI). VI dose-dependently displaced [3H]-15S-(16-m-tolyl)isocarbacyclin on a rat brain slice.

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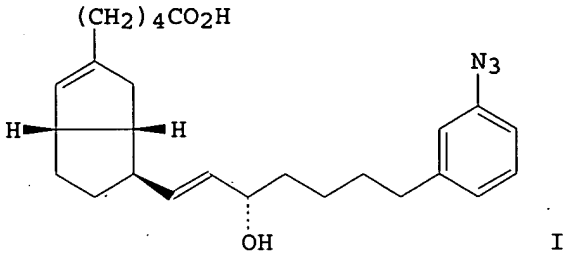

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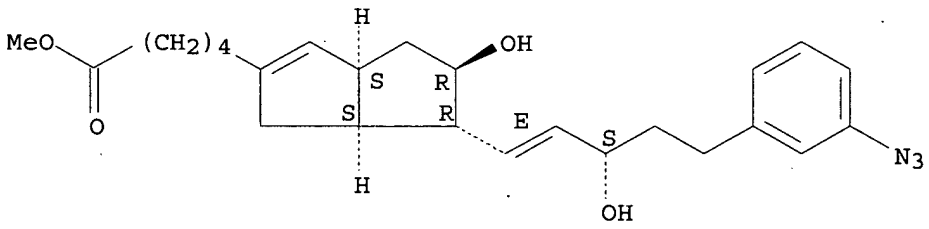
L2 ANSWER 66 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 141978-73-6 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[5-(3-azidophenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H33 N3 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 120:134138 CA
TI Preparation of isocarbacylin derivatives as prostacyclin-like drugs and agents for photoaffinity labeling of proteins
IN Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Negishi, Manabu; Hashimoto, Hitoshi; Ichikawa, Atsushi; Ito, Seiji
PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		

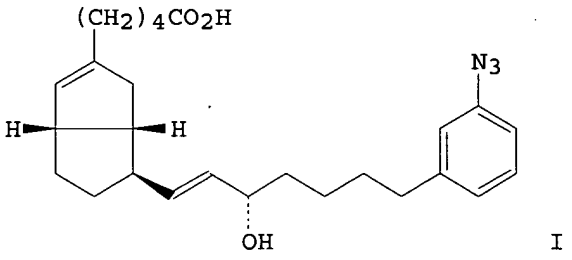
PRAI JP 1991-353175 19911218
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [R1 = H, alkyl; X = H, tritium; Y = H, azido, (trityl)amino; n = 1 - 7] were prepd. Redn. of isocarbacyclin II with [3H]-NaBH4-CeCl3.7H2O (60 Ci/mmol), followed by sapon. and workup, gave isocarbacyclin III. Photoaffinity labeling of PGI2 receptor protein using III indicated that the mol. wt. of the said protein was 43K. Several I showed affinity for prostacyclin receptors.

REFERENCE 2

AN 117:26122 CA
TI An azido-functionalized isocarbacyclin analog acting as an efficient photoaffinity probe for a prostacyclin receptor
AU Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Hashimoto, Hitoshi; Negishi, Manabu; Ichikawa, Atsushi; Ito, Seiji
CS Chem. Instrum. Cent., Nagoya Univ., Chikusa, 464-01, Japan
SO Tetrahedron (1992), 48(13), 2635-58
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
GI



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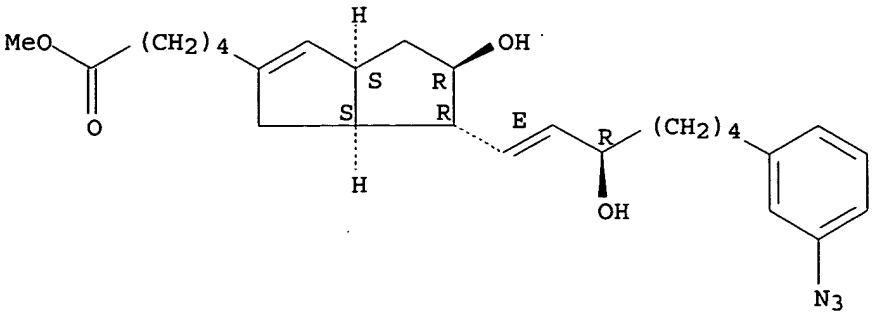
AB A stable prostacyclin analog, I, having an azidophenyl group as a photoaffinity labeling functionality has been synthesized. I has a sufficiently high affinity to the prostacyclin receptor protein in mastocytoma P-815 cells, exhibiting an IC50 value of 3 nM for the replacement of iloprost bound to the receptor protein. A photoaffinity probe compd., [3H]-I, is obtainable by redn. of the ketone with NaB3H4-CeCl3 followed by alk. hydrolysis of the Me ester.

L2 ANSWER 67 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 141887-95-8 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[7-(3-azidophenyl)-3-hydroxy-1-heptenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H37 N3 O4
SR CA
LC STN Files: CA, CAPLUS, CHEMINFORMRX

Absolute stereochemistry.
Double bond geometry as shown.



2 REFERENCES IN FILE CA (1957 TO DATE)
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REFERENCE 1

AN 120:134138 CA
TI Preparation of isocarbacylin derivatives as prostacyclin-like drugs and agents for photoaffinity labeling of proteins
IN Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Negishi, Manabu; Hashimoto, Hitoshi; Ichikawa, Atsushi; Ito, Seiji
PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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SO Tetrahedron (1992), 48(13), 2635-58
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
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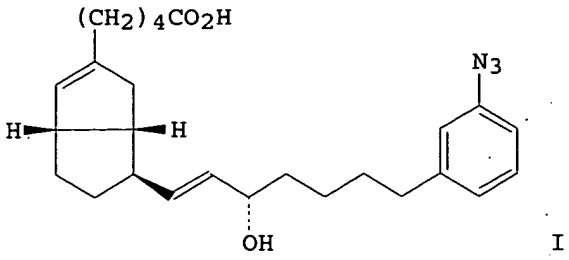
GI



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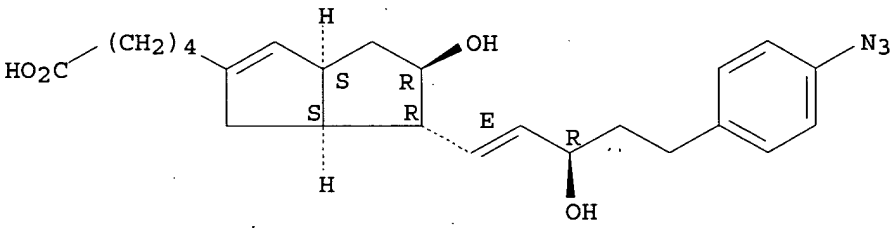
L2 ANSWER 68 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 141887-94-7 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[5-(4-azidophenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H31 N3 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



2 REFERENCES IN FILE CA (1957 TO DATE)
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REFERENCE 1

AN 120:134138 CA
TI Preparation of isocarbacylin derivatives as prostacyclin-like drugs and agents for photoaffinity labeling of proteins
IN Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Negishi, Manabu; Hashimoto, Hitoshi; Ichikawa, Atsushi; Ito, Seiji
PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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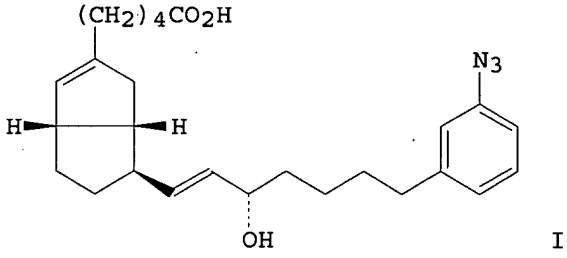
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
GI



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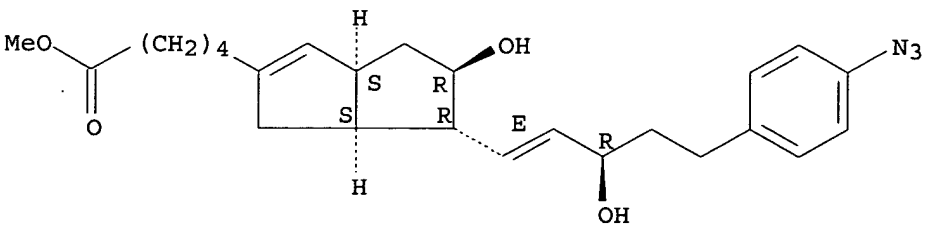
L2 ANSWER 69 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 141887-93-6 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[5-(4-azidophenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H33 N3 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



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AN 120:134138 CA
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PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05163194	A2	19930629	JP 1991-353175	19911218
JP 2872468	B2	19990317		

PRAI JP 1991-353175 19911218
GI

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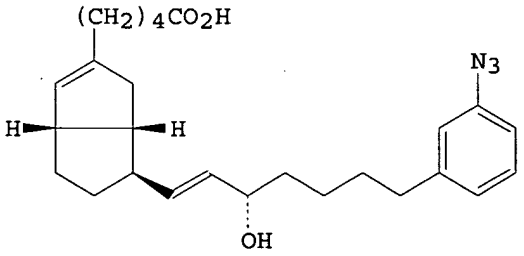
SO Tetrahedron (1992), 48(13), 2635-58
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
GI



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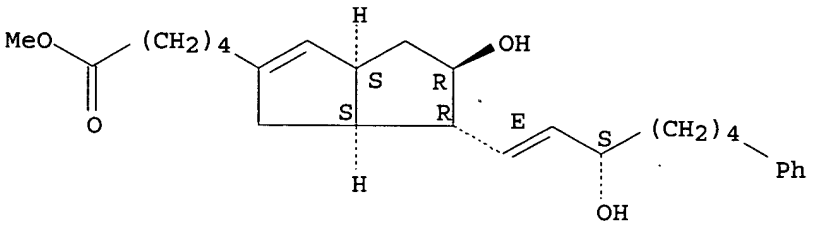
L2 ANSWER 70 OF 78 REGISTRY COPYRIGHT 2003 ACS

RN 141887-83-4 REGISTRY
CN 2-Pentalenepentanoic acid, 1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-(3-hydroxy-7-phenyl-1-heptenyl)-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H38 O4
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 120:134138 CA
TI Preparation of isocarbacylin derivatives as prostacyclin-like drugs and agents for photoaffinity labeling of proteins
IN Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Negishi, Manabu; Hashimoto, Hitoshi; Ichikawa, Atsushi; Ito, Seiji
PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

GI

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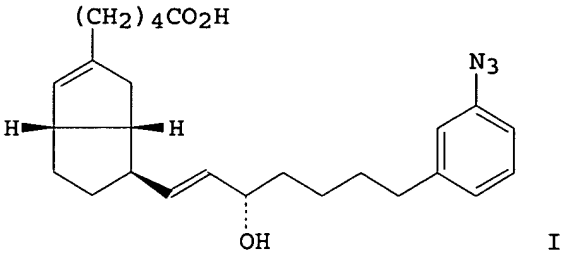
SO Tetrahedron (1992), 48(13), 2635-58
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
GI



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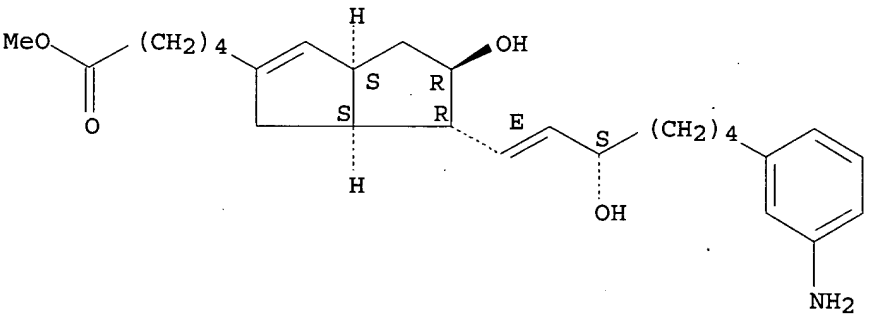
L2 ANSWER 71 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 141887-82-3 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[7-(3-aminophenyl)-3-hydroxy-1-heptenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H39 N O4
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE)
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REFERENCE 1

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CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 05163194	A2	19930629	JP 1991-353175	19911218
JP 2872468	B2	19990317		
PRAI JP 1991-353175		19911218		

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CODEN: TETRAB; ISSN: 0040-4020
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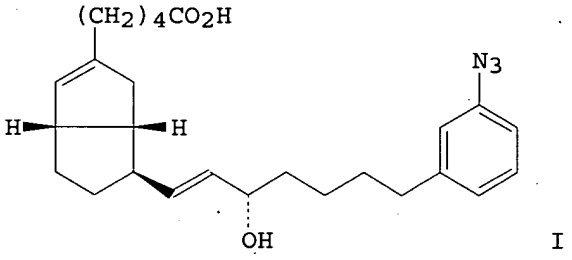

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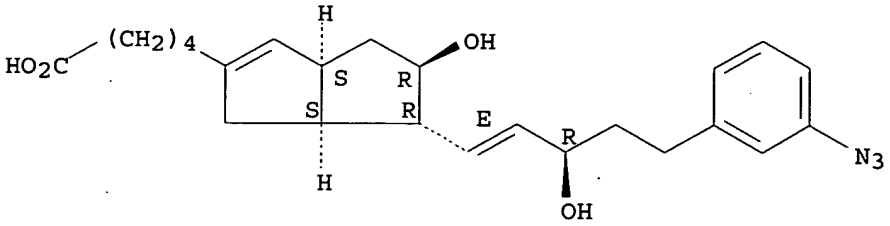
L2 ANSWER 72 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 141887-81-2 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[5-(3-azidophenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H31 N3 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as shown.



1 REFERENCES IN FILE CA (1957 TO DATE)
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REFERENCE 1

AN 117:26122 CA
TI An azido-functionalized isocarbacyclin analog acting as an efficient photoaffinity probe for a prostacyclin receptor
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CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
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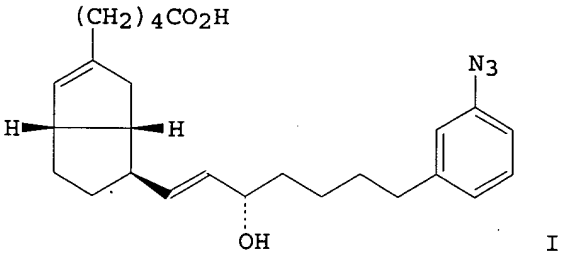

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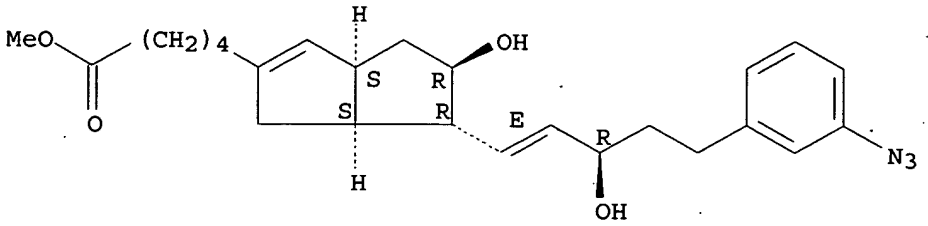
L2 ANSWER 73 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 141887-80-1 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[5-(3-azidophenyl)-3-hydroxy-1-pentenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H33 N3 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 120:134138 CA
TI Preparation of isocarbacylin derivatives as prostacyclin-like drugs and agents for photoaffinity labeling of proteins
IN Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Negishi, Manabu; Hashimoto, Hitoshi; Ichikawa, Atsushi; Ito, Seiji
PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

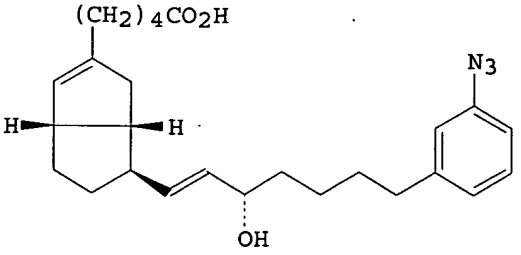
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [R1 = H, alkyl; X = H, tritium; Y = H, azido, (trityl)amino; n = 1 - 7] were prepd. Redn. of isocarbacyclin II with [3H]-NaBH4-CeCl3.7H2O (60 Ci/mmol), followed by sapon. and workup, gave isocarbacyclin III. Photoaffinity labeling of PGI2 receptor protein using III indicated that the mol. wt. of the said protein was 43K. Several I showed affinity for prostacyclin receptors.

REFERENCE 2

AN 117:26122 CA
TI An azido-functionalized isocarbacyclin analog acting as an efficient photoaffinity probe for a prostacyclin receptor
AU Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Hashimoto, Hitoshi; Negishi, Manabu; Ichikawa, Atsushi; Ito, Seiji
CS Chem. Instrum. Cent., Nagoya Univ., Chikusa, 464-01, Japan
SO Tetrahedron (1992), 48(13), 2635-58
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
GI



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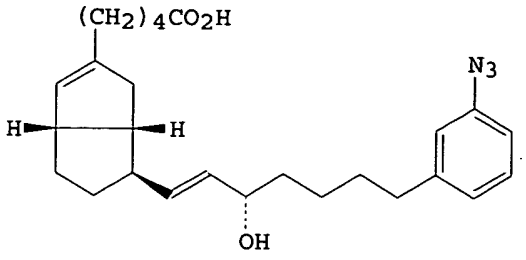
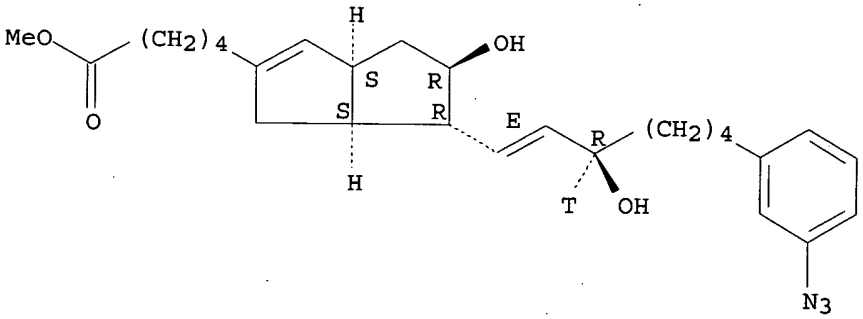


I

AB A stable prostacyclin analog, I, having an azidophenyl group as a photoaffinity labeling functionality has been synthesized. I has a sufficiently high affinity to the prostacyclin receptor protein in mastocytoma P-815 cells, exhibiting an IC50 value of 3 nM for the replacement of iloprost bound to the receptor protein. A photoaffinity probe compd., [3H]-I, is obtainable by redn. of the ketone with NaB3H4-CeCl3 followed by alk. hydrolysis of the Me ester.

L2 ANSWER 74 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 141887-73-2 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[7-(3-azidophenyl)-3-hydroxy-1-heptenyl-3-t]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, methyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3S*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H36 N3 O4 T
SR CA
LC STN Files: CA, CAPLUS

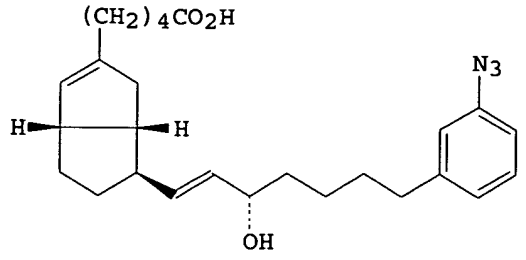
Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 117:26122 CA
TI An azido-functionalized isocarbacyclin analog acting as an efficient photoaffinity probe for a prostacyclin receptor
AU Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Hashimoto, Hitoshi; Negishi, Manabu; Ichikawa, Atsushi; Ito, Seiji
CS Chem. Instrum. Cent., Nagoya Univ., Chikusa, 464-01, Japan
SO Tetrahedron (1992), 48(13), 2635-58
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
GI

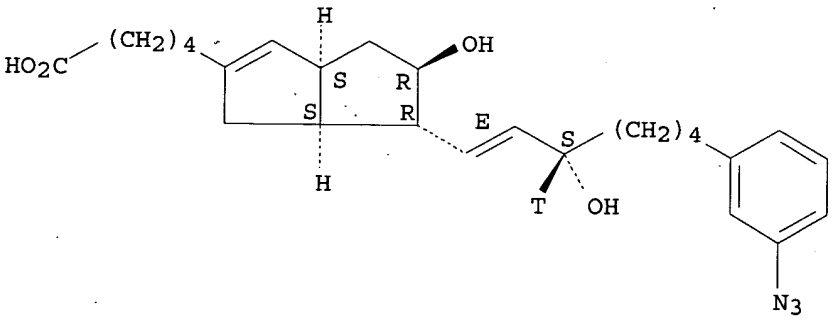


I

AB A stable prostacyclin analog, I, having an azidophenyl group as a photoaffinity labeling functionality has been synthesized. I has a sufficiently high affinity to the prostacyclin receptor protein in mastocytoma P-815 cells, exhibiting an IC50 value of 3 nM for the replacement of iloprost bound to the receptor protein. A photoaffinity probe compd., [3H]-I, is obtainable by redn. of the ketone with NaB3H4-CeCl3 followed by alk. hydrolysis of the Me ester.

L2 ANSWER 75 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 140900-72-7 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[7-(3-azidophenyl)-3-hydroxy-1-heptenyl-3-t]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H34 N3 O4 T
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



3 REFERENCES IN FILE CA (1957 TO DATE)
3 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 120:134138 CA
TI Preparation of isocarbacylin derivatives as prostacyclin-like drugs and agents for photoaffinity labeling of proteins
IN Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Negishi, Manabu; Hashimoto, Hitoshi; Ichikawa, Atsushi; Ito, Seiji
PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

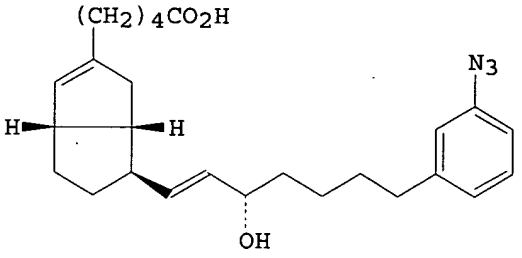
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [R1 = H, alkyl; X = H, tritium; Y = H, azido, (trityl)amino; n = 1 - 7] were prepd. Redn. of isocarbacyclin II with [3H]-NaBH4-CeCl3.7H2O (60 Ci/mmol), followed by sapon. and workup, gave isocarbacyclin III. Photoaffinity labeling of PGI2 receptor protein using III indicated that the mol. wt. of the said protein was 43K. Several I showed affinity for prostacyclin receptors.

REFERENCE 2

AN 117:26122 CA
TI An azido-functionalized isocarbacyclin analog acting as an efficient photoaffinity probe for a prostacyclin receptor
AU Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Hashimoto, Hitoshi; Negishi, Manabu; Ichikawa, Atsushi; Ito, Seiji
CS Chem. Instrum. Cent., Nagoya Univ., Chikusa, 464-01, Japan
SO Tetrahedron (1992), 48(13), 2635-58
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
GI



I

AB A stable prostacyclin analog, I, having an azidophenyl group as a photoaffinity labeling functionality has been synthesized. I has a sufficiently high affinity to the prostacyclin receptor protein in mastocytoma P-815 cells, exhibiting an IC50 value of 3 nM for the replacement of iloprost bound to the receptor protein. A photoaffinity probe compd., [3H]-I, is obtainable by redn. of the ketone with NaB3H4-CeCl3 followed by alk. hydrolysis of the Me ester.

REFERENCE 3

AN 116:228877 CA
TI Study on the structure of a prostacyclin receptor protein. Identification of the molecular weight by photoaffinity labeling method
AU Suzuki, M.; Koyano, H.; Noyori, R.; Hashimoto, H.; Negishi, M.; Ichikawa, A.; Ito, S.
CS Chem. Instrum. Cent., Nagoya Univ., Nagoya, Japan
SO Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1991), 33rd, 691-8
CODEN: TYKYDS
DT Journal
LA Japanese
GI

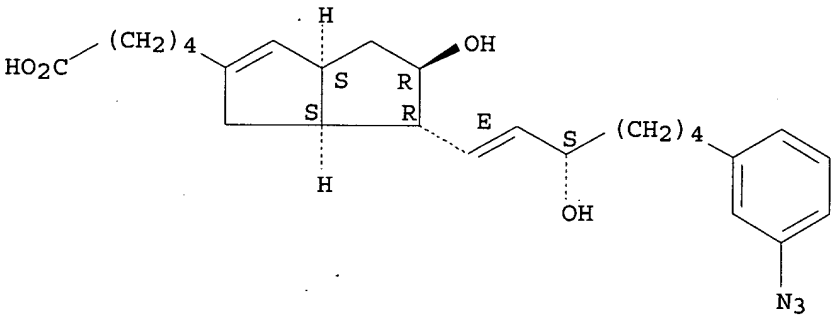
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The azidophenyl deriv., I, has been synthesized by structural modification of isocarbacyclin Me ester II. First, the C(13)-C(14) double bond of II is selectively epoxidized by Sharpless epoxidn. giving III whose 11- and

15-hydroxyl groups are acetylated. Epoxy ring opening of resulting IV with ArYt-H2O and subsequent deacetylation with aq. K2CO3 and cleaved with NaIO4 to give an aldehyde. Horner-Emmons reaction with V gives an enone (VI) which was reduced with NaBH4-CeCl3 is followed by sepn. of the resulting 15-epimers and alk. hydrolysis of the Me ester to give I. This compd. exhibits high affinity to the PGI2 receptor protein(s) in mastocytoma P-815 cells with the IC50 value of 3 nM. The tritium labeled deriv., [3H]-I, synthesized by redn. of VI with [3H]NaBH4-CeCl3 followed by alk. hydrolysis, has been used for the photoaffinity labeling expt. Plasma membrane fraction of mastocytoma P-815 cells which is abundant in the PGI2 receptor protein(s) is incubated with [3H] I and then irradiated with a UV lamp. The irradiated material is subjected to SDS-PAGE and fluorog. showing a clear band around 43 k. The photoreaction in presence of GTP-.gamma.S decreases the intensity of this band. The addn. of iloprost to the incubated media completely suppresses the formation of this band. These results confirm the mol. wt. of the PGI2 receptor protein(s) in mastocytoma P-815 cells to be 43 k.

L2 ANSWER 76 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 140900-65-8 REGISTRY
CN 2-Pentalenepentanoic acid, 6-[7-(3-azidophenyl)-3-hydroxy-1-heptenyl]-1,3a,4,5,6,6a-hexahydro-5-hydroxy-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H35 N3 O4
SR CA
LC STN Files: CA, CANCERLIT, CAPLUS, CHEMINFORMRX, MEDLINE

Absolute stereochemistry.
Double bond geometry as shown.



5 REFERENCES IN FILE CA (1957 TO DATE)
5 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 122:9691 CA
TI Unnatural prostaglandins of biochemical and physiological significance
AU Noyori, R.; Koyano, H.; Mori, M.; Hirata, R.; Shiga, Y.; Kokura, T.; Suzuki, M.
CS Dep. of Chemistry, Nagoya Univ., Nagoya, 464-01, Japan
SO Pure and Applied Chemistry (1994), 66(10/11), 1999-2005
CODEN: PACHAS; ISSN: 0033-4545
DT Journal; General Review
LA English
AB A review with 15 refs. Some artificial prostaglandins (PGs) synthesized by the three-component process possess significant biol. properties. Isocarbacyclin, a stable analog of PGI2, is a promising agent for the treatment of various thrombotic diseases. 19-(3-Azidophenyl)-20-norisocarbacyclin (APNIC) has a sufficiently high affinity to the prostacyclin receptor protein in mastocytomas P-815 cells, exhibiting an IC50 value of 3 nM for the replacement of iloprost. Photoaffinity labeling expts. using 15-tritium-labeled APNIC have resulted in the characterization of the PGI2 receptor protein. .DELTA.7-PGA1 Me ester exhibits unique anti-tumor and anti-viral activities independent of cAMP levels. The dienone PGs are transported reversibly into cultured L1210

leukemia cells and then accumulate in nuclei via covalent interaction, eliciting growth inhibition. This cellular behavior is well correlated with the chem. behavior in the presence of thiols. The dienone undergoes a reversible Michael reaction with various thiols in the homogeneous phase, whereas the reaction with polymer-anchored thiols occurs in an irreversible manner. PGA1 Me ester, a less potent enone PG, reacts with thiols at a lower rate, but the resulting adducts are more stable than the dienone adducts.

REFERENCE 2

AN 120:134138 CA
TI Preparation of isocarbacylin derivatives as prostacyclin-like drugs and agents for photoaffinity labeling of proteins
IN Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Negishi, Manabu; Hashimoto, Hitoshi; Ichikawa, Atsushi; Ito, Seiji
PA Teijin Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05163194	A2	19930629	JP 1991-353175	19911218
	JP 2872468	B2	19990317		
PRAI	JP 1991-353175		19911218		

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [R1 = H, alkyl; X = H, tritium; Y = H, azido, (trityl)amino; n = 1 - 7] were prepd. Redn. of isocarbacyclin II with [3H]-NaBH4-CeCl3.7H2O (60 Ci/mmol), followed by sapon. and workup, gave isocarbacyclin III. Photoaffinity labeling of PGI2 receptor protein using III indicated that the mol. wt. of the said protein was 43K. Several I showed affinity for prostacyclin receptors.

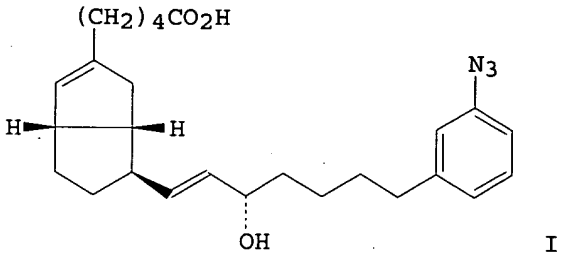
REFERENCE 3

AN 117:143609 CA
TI Identification of the prostacyclin receptor by use of [15-3H1]-19-(3-azidophenyl)-20-norisocarbacyclin, an irreversible specific photoaffinity probe
AU Ito, Seiji; Hashimoto, Hitoshi; Negishi, Manabu; Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Ichikawa, Atsushi
CS Dep. Cell Biol., Osaka Biosci. Inst., Suita, 565, Japan
SO Journal of Biological Chemistry (1992), 267(28), 20326-30
CODEN: JBCHA3; ISSN: 0021-9258
DT Journal
LA English
AB The PGI2 receptor of mouse mastocytoma P-815 cells was characterized by photoaffinity labeling with the stable PGI2 analog [15-3H1]-19-(3-azidophenyl)-9(O)-methano-.DELTA.6(9.alpha.)-20-nor-PGI1([3H]APNIC) used as a potential photoaffinity probe for the receptor. [3H]APNIC bound to the mastocytoma membrane with high affinity and in a saturable manner. Scatchard plot anal. indicated a single binding site with a KD of 4.7 nM and a Bmax of 0.58 pmol/mg protein. The binding of [3H]APNIC was dose dependently inhibited by APNIC and iloprost, another stable PGI2 agonist, and to a much lesser extent by PGE2. The binding of the radioligand showed sensitivity to the guanine nucleotide GTP.gamma.S. Photolysis of [3H]APNIC-prelabeled membranes resulted in incorporation of radiolabeled into a protein of approx. 43 kDa. Photolabeling was inhibited by PGI2 agonists and other prostaglandins with specificity for the PGI2 receptor and was modulated by GTP.gamma.S. A protein of approx. 45 kDa was also labeled by [3H]APNIC in the membrane of porcine platelets, membranes that

are known to be abundant in PGI2 receptors. These results demonstrate that [3H]APNIC specifically labels a protein that may represent the PGI2 receptor and that this radioprobe will be a useful reagent for further characterization and purifn. of the PGI2 receptor.

REFERENCE 4

AN 117:26122 CA
TI An azido-functionalized isocarbacyclin analog acting as an efficient photoaffinity probe for a prostacyclin receptor
AU Suzuki, Masaaki; Koyano, Hiroshi; Noyori, Ryoji; Hashimoto, Hitoshi; Negishi, Manabu; Ichikawa, Atsushi; Ito, Seiji
CS Chem. Instrum. Cent., Nagoya Univ., Chikusa, 464-01, Japan
SO Tetrahedron (1992), 48(13), 2635-58
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
GI



I

AB A stable prostacyclin analog, I, having an azidophenyl group as a photoaffinity labeling functionality has been synthesized. I has a sufficiently high affinity to the prostacyclin receptor protein in mastocytoma P-815 cells, exhibiting an IC50 value of 3 nM for the replacement of iloprost bound to the receptor protein. A photoaffinity probe compd., [3H]-I, is obtainable by redn. of the ketone with NaB3H4-CeCl3 followed by alk. hydrolysis of the Me ester.

REFERENCE 5

AN 116:228877 CA
TI Study on the structure of a prostacyclin receptor protein. Identification of the molecular weight by photoaffinity labeling method
AU Suzuki, M.; Koyano, H.; Noyori, R.; Hashimoto, H.; Negishi, M.; Ichikawa, A.; Ito, S.
CS Chem. Instrum. Cent., Nagoya Univ., Nagoya, Japan
SO Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1991), 33rd, 691-8
CODEN: TYKYDS
DT Journal
LA Japanese
GI

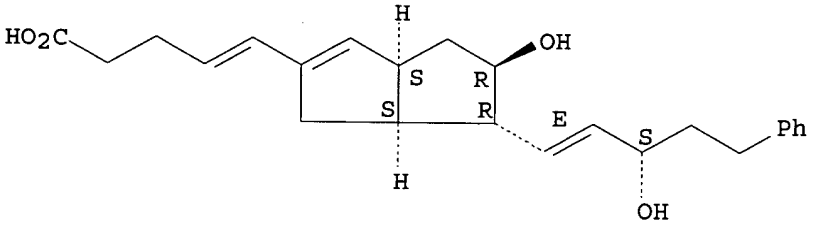
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The azidophenyl deriv., I, has been synthesized by structural modification of isocarbacyclin Me ester II. First, the C(13)-C(14) double bond of II is selectively epoxidized by Sharpless epoxidn. giving III whose 11- and 15-hydroxyl groups are acetylated. Epoxy ring opening of resulting IV with ArYt-H2O and subsequent deacetylation with aq. K2CO3 and cleaved with NaIO4 to give an aldehyde. Horner-Emmons reaction with V gives an enone (VI) which was reduced with NaBH4-CeCl3 is followed by sepn. of the resulting 15-epimers and alk. hydrolysis of the Me ester to give I. This compd. exhibits high affinity to the PGI2 receptor protein(s) in mastocytoma P-815 cells with the IC50 value of 3 nM. The tritium labeled

deriv., [3H]-I, synthesized by redn. of VI with [3H]NaBH4-CeCl3 followed by alk. hydrolysis, has been used for the photoaffinity labeling expt. Plasma membrane fraction of mastocytoma P-815 cells which is abundant in the PGI2 receptor protein(s) is incubated with [3H] I and then irradiated with a UV lamp. The irradiated material is subjected to SDS-PAGE and fluorog. showing a clear band around 43 k. The photoreaction in presence of GTP-.gamma.S decreases the intensity of this band. The addn. of iloprost to the incubated media completely suppresses the formation of this band. These results confirm the mol. wt. of the PGI2 receptor protein(s) in mastocytoma P-815 cells to be 43 k.

L2 ANSWER 77 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 102637-66-1 REGISTRY
CN 4-Pentenoic acid, 5-[1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-(3-hydroxy-5-phenyl-1-pentenyl)-2-pentalenyl]-, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H30 O4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry as described by E or Z.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

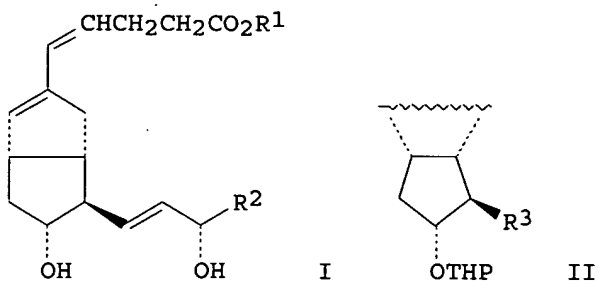
2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 107:197933 CA
TI Prostaglandin I2 analogs and pharmaceutical compositions containing them
IN Shibazaki, Masakatsu; Sodeoka, Mikiko; Izeki, Katsuhiko; Shinoda, Maki; Ishama, Choko; Hayashi, Yoshio; Kanayama, Toshimoto
PA Sagami Chemical Research Center, Japan; Mitsubishi Petrochemical Co., Ltd.
SO Jpn. Kokai Tokkyo Koho, 24 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 62029548	A2	19870207	JP 1985-167681	19850731
	JP 04055416	B4	19920903		
	CA 1280112	A1	19910212	CA 1986-515127	19860731
	US 5053526	A	19911001	US 1990-511945	19900416
PRAI	JP 1984-165669	19840809			
	JP 1985-167681	19850731			
	US 1985-763618	19850808			
	US 1987-99779	19870922			
	US 1988-206943	19880613			
	US 1989-333733	19890403			

GI



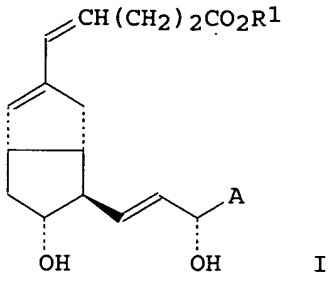
AB The title compds. [E or Z-I; R1 = H, C1-12 alkyl, cycloalkyl, Ph; R2 = cyclohexyl, CHMeCH2C.tplbond.CEt, CH2CHMeC.tplbond.CEt, CH2CHMeC.tplbond.CEt, CHMe(CH2)4Me, PhCH2CH2, CMe2(CH2)3Me, CH2CHMeCH2CH2Me, 2-methylhexyl], which show blood platelet aggregation-inhibitory, antihypertensive, vasodilating and antiulcer activities and are useful as antithrombotics and antiulcer agents, were prepd. Oxidn. of a bicyclo[3,3,0]oct-2-ene deriv. (II; THP = tetrahydropyranyl, R1 = Et, R3 = CH2OH) with SO3-pyridine in DMSO contg. Et3N and reaction of the resulting II (R3 = CHO) with (3S)-EtC.tplbond.CCH2CHMeCOCH2P(O)(OMe)2 in the presence of NaH gave 86% II [R1 = Et, R3 = (3S)-CH:CHCOCHMeCH2C.tplbond.CEt] which was reduced with NaBH4 in MeOH at -40.degree. to -20.degree. and then deprotected by 65% aq. AcOH to give 46% I (R1 = Et, R2 = (1S)-CHMeCH2.tplbond.CEt]. I in vitro inhibited human blood platelet aggregation with an IC50 of 6 .times. 10-10-2 .times. 10-7M and at 100 .mu.g/kg reduced by 18.1-89.9% stomach acid secretion in rats. Tablets contg. I, CM-cellulose Ca salt, SiO2, Mg stearate and mannitol were prepd.

REFERENCE 2

AN 105:12115 CA
TI Pharmaceuticals containing prostaglandin I2
IN Ishibashi, Akira; Horii, Daijiro; Kanayama, Toshiji; Iseki, Katsuhiko; Shinoda, Masaki; Ishiyama, Chiyoko; Hayashi, Yosio; Shibasaki, Masakatsu; Sodeoka, Mikiko; et al.
PA Mitsubishi Yuka Pharmaceutical Co., Ltd., Japan; Sagami Chemical Research Center
SO Eur. Pat. Appl., 57 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 171992	A2	19860219	EP 1985-305611	19850807
	EP 171992	A3	19861203		
	EP 171992	B1	19900606		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	JP 61044819	A2	19860304	JP 1984-165669	19840809
	JP 02044452	B4	19901004		
	AT 53295	E	19900615	AT 1985-305611	19850807
	US 4699921	A	19871013	US 1985-763618	19850808
PRAI	JP 1984-165669	19840809			
	EP 1985-305611	19850807			

GI

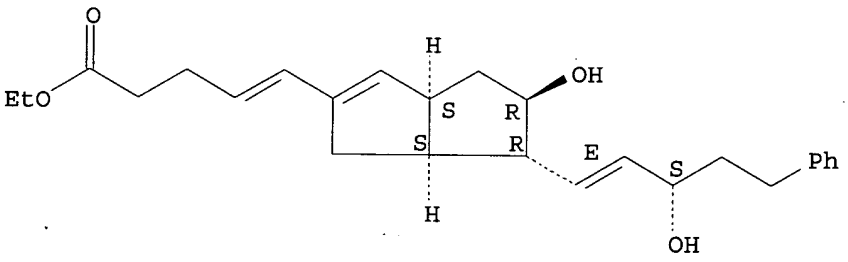


I

AB Pharmaceuticals contg. prostaglandin I2 analogs I, where R1 = H, C1-12 alkyl, C4-7 cycloalkyl, or Ph and A = pentyl, cyclopentyl, cyclohexyl, etc., or a nontoxic salt or cyclodextrin inclusion compd. thereof have circulation ameliorating and antiulcer effects. The synthesis, formation, and biol. activity of I were described. E.g., 3-(4-methoxycarbonyl-1-butenyl)-6S-(3-oxo-trans-1-octenyl)-7R-tetrahydropyranyloxy-1S,5S-cis-bicyclo[3.3.0]oct-2-ene was reduced to the corresponding 6S-(3RS-hydroxy) deriv. with NaBH4 and the latter compd. hydrolyzed and subjected to silica gel chromatog. to afford 3-(4-methoxycarbonyl-1-butenyl)-6S-(3S-hydroxy-trans-1-octenyl)-7R-hydroxy-1S,5S-cis-bicyclo[3.3.0]oct-2-ene (II). II (5 mg) was dissolved in 5 mL EtOH and mixed with 0.2 g Ca CM-cellulose, 20 mg SiO2, 0.2 g Mg stearate, and 5 g mannitol. After drying the mixt. was made to 10 g with mannitol and tabletted (100 tablets). The free acid of II (3 mg/kg, i.v.) decreased blood pressure 43% in anesthetized rats.

L2 ANSWER 78 OF 78 REGISTRY COPYRIGHT 2003 ACS
RN 102637-57-0 REGISTRY
CN 4-Pentenoic acid, 5-[1,3a,4,5,6,6a-hexahydro-5-hydroxy-6-(3-hydroxy-5-phenyl-1-pentenyl)-2-pentalenyl]-, ethyl ester, [3aS-[3a.alpha.,5.beta.,6.alpha.(1E,3R*),6a.alpha.]]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H34 O4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry as described by E or Z.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

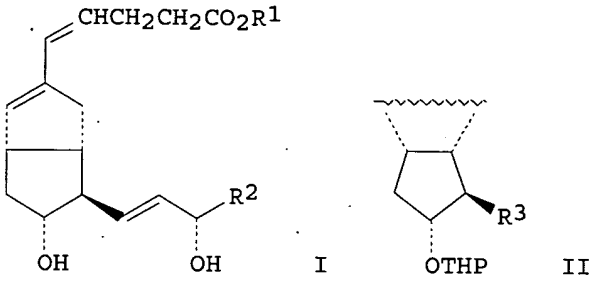
REFERENCE 1

AN 107:197933 CA
TI Prostaglandin I2 analogs and pharmaceutical compositions containing them
IN Shibazaki, Masakatsu; Sodeoka, Mikiko; Izeki, Katsuhiko; Shinoda, Maki; Ishama, Choko; Hayashi, Yoshio; Kanayama, Toshimoto
PA Sagami Chemical Research Center, Japan; Mitsubishi Petrochemical Co., Ltd.
SO Jpn. Kokai Tokkyo Koho, 24 pp.
CODEN: JKXXAF
DT Patent
LA Japanese

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 62029548	A2	19870207	JP 1985-167681	19850731
	JP 04055416	B4	19920903		
	CA 1280112	A1	19910212	CA 1986-515127	19860731
	US 5053526	A	19911001	US 1990-511945	19900416
PRAI	JP 1984-165669	19840809			
	JP 1985-167681	19850731			
	US 1985-763618	19850808			
	US 1987-99779	19870922			
	US 1988-206943	19880613			
	US 1989-333733	19890403			

GI



AB The title compds. [E or Z-I; R1 = H, C1-12 alkyl, cycloalkyl, Ph; R2 = cyclohexyl, CHMeCH2C.tplbond.CEt, CH2CHMeC.tplbond.CEt, CH2CHMeC.tplbond.CEt, CHMe(CH2)4Me, PhCH2CH2, CMe2(CH2)3Me, CH2CHMeCH2CH2Me, 2-methylhexyl], which show blood platelet aggregation-inhibitory, antihypertensive, vasodilating and antiulcer activities and are useful as antithrombotics and antiulcer agents, were prepd. Oxidn. of a bicyclo[3,3,0]oct-2-ene deriv. (II; THP = tetrahydropyranyl, R1 = Et, R3 = CH2OH) with SO3-pyridine in DMSO contg. Et3N and reaction of the resulting II (R3 = CHO) with (3S)-EtC.tplbond.CCH2CHMeCOCH2P(O)(OMe)2 in the presence of NaH gave 86% II [R1 = Et, R3 = (3S)-CH:CHCOCHMeCH2C.tplbond.CEt] which was reduced with NaBH4 in MeOH at -40.degree. to -20.degree. and then deprotected by 65% aq. AcOH to give 46% I (R1 = Et, R2 = (1S)-CHMeCH2.tplbond.CEt]. I in vitro inhibited human blood platelet aggregation with an IC50 of 6 .times. 10-10-2 .times. 10-7M and at 100 .mu.g/kg reduced by 18.1-89.9% stomach acid secretion in rats. Tablets contg. I, CM-cellulose Ca salt, SiO2, Mg stearate and mannitol were prepd.

REFERENCE 2

AN 105:12115 CA
TI Pharmaceuticals containing prostaglandin I2
IN Ishibashi, Akira; Horii, Daijiro; Kanayama, Toshiji; Iseki, Katsuhiko; Shinoda, Masaki; Ishiyama, Chiyoko; Hayashi, Yosio; Shibasaki, Masakatsu; Sodeoka, Mikiko; et al.
PA Mitsubishi Yuka Pharmaceutical Co., Ltd., Japan; Sagami Chemical Research Center
SO Eur. Pat. Appl., 57 pp.
CODEN: EPXXDW
DT Patent
LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 171992	A2	19860219	EP 1985-305611	19850807
	EP 171992	A3	19861203		
	EP 171992	B1	19900606		

R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE

	JP 61044819	A2	19860304	JP 1984-165669	19840809
	JP 02044452	B4	19901004		
	AT 53295	E	19900615	AT 1985-305611	19850807
	US 4699921	A	19871013	US 1985-763618	19850808
PRAI	JP 1984-165669	19840809			
	EP 1985-305611	19850807			

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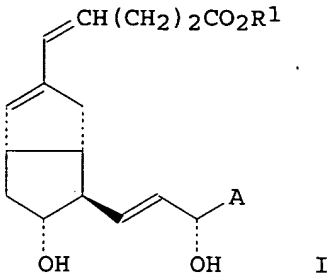

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